A “figure of merit” for susceptibility of irradiated amorphous metal alloys to thermal spike-induced plasticity

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Thermal spikes in irradiated amorphous metal alloys emit stress pulses of sufficient intensity to trigger plastic deformation in adjacent unmelted material. This localized plasticity may lead to macro-scale anisotropic shape changes in metallic glasses under neutron or ion irradiation, even in the absence of external loading. We formulate a micromechanical model that connects thermal spike-induced plasticity (TSIP) to bulk properties of amorphous metal alloys. This model gives rise to a “figure of merit” (FOM) for ranking the susceptibility of metallic glasses to TSIP without recourse to further experiments or simulations. We validate the FOM against molecular dynamics simulations of TSIP in amorphous Cu-Nb alloys.

Keywords: Radiation effects; metallic glasses; molecular dynamics; plasticity

1. Introduction

Metallic glasses are a class of alloys with disordered atomic-level structure [1, 2]. The effect of this structure on properties has been widely investigated, especially as it relates to the distinctive mechanical behavior of metallic glasses [3, 4]. The non-crystalline structure of metallic glasses may also account for major differences between the radiation response of these materials and that of crystalline alloys. For example, while crystalline alloys swell without limit under continuous irradiation [5, 6], amorphous materials may expand or contract following irradiation [7]. Moreover, radiation induced density changes appear to saturate in some metallic glasses [8]. Irradiation generally embrittles crystalline alloys [9], but some irradiated amorphous alloys become more ductile [10, 11, 12]. Finally, irradiation by swift heavy ions with energies in the electronic stopping regime gives rise to the “ion hammer” effect: anisotropic shape change in the absence of applied external loads [13]. No analogous phenomenon has been observed in crystalline metals.¹

In the present work, we construct a mechanistic model for one distinctive radiation response of amorphous metal alloys, recently predicted using large-scale molecular dynamics simulations: thermal-spike induced plasticity (TSIP) [16]. TSIP occurs because rapid melting within thermal spikes produces stress pulses of sufficient amplitude to trigger plastic deformation in surrounding, unmelted material. Since TSIP arises due to thermal spikes induced by inter-nuclear collisions, it is distinct from the ion hammer effect. In particular, TSIP may occur under

¹ Radiation-induced anisotropic growth in low-symmetry crystalline metals [14, 15], such as Zr-base alloys, is mechanistically distinct from the ion hammer effect [13].

conditions where the majority of the kinetic energy of incident particles is lost to nuclear—rather than electronic—stopping, such as neutron or low energy ($<0.5\text{MeV}$) ion irradiation.

TSIP may cause macroscale anisotropic shape changes in metallic glasses irradiated by unidirectional particle beams, even when no external loads are applied. It therefore has important consequences for potential applications of metallic glasses under irradiation: deleterious in some cases (e.g. dimensional changes in structural components) and beneficial in others (e.g. in radiation sensing or radiation-induced actuation) [16]. In this Article we formulate a micromechanical model for TSIP in metallic glasses through application of continuum solid mechanics and thermodynamics. This physics-based model relates TSIP to bulk material properties and may therefore be thought of as a “figure of merit” (FOM) for screening candidate alloys for specific applications. It may also be used to design experiments intended to validate our modeling predictions concerning TSIP.

In the following section, we summarize our previous findings on the TSIP mechanism. Next, we present a complete derivation of the micromechanical model for TSIP. Finally, we validate the micromechanical model through comparison with six large-scale molecular dynamics simulations described previously [17]. The good agreement between these simulations and our model shows that the micromechanical model presented here is a useful tool for tailoring the radiation response of amorphous metal alloys.

2. Thermal spike induced plasticity (TSIP) mechanism

Fig. 1 summarizes our previous findings on the atomic-scale radiation response mechanisms of metallic glasses leading to TSIP. The process begins with the dissipation of kinetic energy from a primary knock-on atom (PKA) via nuclear stopping in a volume on the order of $\sim 10\text{ nm}$ in diameter. As shown in Fig. 1(a), this step lasts $\sim 0.3\text{ ps}$. Within $\sim 1\text{ ps}$, the

energy deposited by the PKA comes to thermal equilibrium in the ~ 10 nm diameter volume, leading to localized heating above the glass transition temperature and the formation of a thermal spike (TS) [Fig. 1(b)]. The core of the TS is an equilibrium liquid, with identical diffusion kinetics and thermodynamic properties to a bulk equilibrium liquid of the same composition, temperature, and pressure [17]. However, the thermal expansion of the liquid in a TS is constrained by the surrounding unmelted material, leading to rapid TS pressurization and production of an intense stress pulse on times between 1-2 ps [Fig. 1(c)]. This stress pulse travels away from the TS at the longitudinal speed of sound.

TSIP occurs when the stress pulse is of sufficient intensity to trigger plastic deformation in surrounding, unmelted material [16]. While TSs tend to be ellipsoidal at the moment of their formation [Fig. 1(b) and 1(c)], plastic deformation in the surrounding material drives them toward a more spherical shape. This tendency to transform from ellipsoidal to spherical may be described by a specific form of the deviatoric plastic strain tensor: compressive in the radial and axial directions and tensile in the hoop direction. TSIP occurs on times of ~ 2 -3 ps [Fig. 1(d)]. Finally over times exceeding 10 ps, heat is conducted away from the TS, cooling the TS core at rates $> 10^{13}$ K/s. In glass-forming solids, such a high quench rate leads to vitrification of the TS core into a glassy inclusion of exceptionally high fictive temperature, which we termed a “super-quenched zone” (SQZ) [Fig. 1(e)] [17].

3. A figure of merit for TSIP

3.1 Mechanistic rationale

The qualitative mechanistic model given in the previous section leads us to propose a quantitative “figure of merit” (FOM) for TSIP, i.e. a parameter, χ , for ranking the relative susceptibility of different amorphous metal alloys to TSIP. TSIP occurs when the vitrified solid

adjacent to a thermal spike (TS) undergoes plastic deformation. If the stress pulse generated by the TS does not exceed the yield stress anywhere in the surrounding solid matrix, no TSIP takes place. On the other hand, if the yield stress in the matrix is exceeded, the extent of the ensuing plastic deformation depends on the flow rule of the material and is expected to increase with the intensity of the stress pulse. Therefore, we construct and assess a FOM χ defined as the ratio of the maximum von Mises stress in the unmelted material adjacent to the TS, σ_{vM}^{max} , to the yield stress of the amorphous alloy, σ_Y :

$$\chi = \sigma_{vM}^{max} / \sigma_Y.$$

(EQ 1)

When $\chi < 1$, this FOM predicts no TSIP. For $\chi > 1$, the amount of TSIP is expected to increase with increasing χ .

χ is preferably to be formulated in such a way that predictions concerning the relative TSIP susceptibilities of different amorphous metal alloys may be made without having to conduct dedicated irradiation experiments or simulations for each alloy. Thus, it is of interest to express χ in terms of materials properties that may be more easily measured or calculated. Yield stress, σ_Y , is such a property. By contrast, σ_{vM}^{max} is not a materials property, but rather the outcome of the TS process itself. We therefore construct a model that relates σ_{vM}^{max} to materials properties.

To formulate this model, we neglect the initially ellipsoidal shape of TSs and instead use the solution for time-dependent elastic fields in material surrounding a spherical TS. As we showed previously [16], the only consequence of the ellipsoidal TS shape is the polarity of plastic strain field. The shape does not have a strong effect on the magnitude of the stress and so we approximate TSs as spheres in the present work. Therefore, the TS itself is treated as a

spherical cavity of radius a initially at equilibrium with its surroundings and pressurized suddenly to pressure P at $t = 0$. The cavity is embedded in an infinite elastic medium. Under these assumptions, the displacement field in material adjacent to a TS is purely radial and described by a time-dependent analytical solution [18].

Using this simplified micromechanical model, we complete the expression for χ in three steps:

1. We use isotropic linear elasticity to compute the strain and stress fields adjacent to a spherical TS, yielding an analytical expression for $\sigma_{vM}(r, t)$.
2. We evaluate for the maximum value of $\sigma_{vM}(r, t)$ and find that it occurs at the interface of the TS and adjacent unmelted material and is a function of the maximum pressure in the TS, $\sigma_{vM}^{max} = f(P_{max})$
3. We develop a thermodynamic model to predict the maximum pressure P_{max} in the TS.

Each of these steps is described in the following three sections. Putting all of the components of the model together, we obtain an expression for χ in terms of material properties alone. We validate this FOM in Section 4 by comparing it with TSIP predictions obtained from molecular dynamics simulations.

3.2 Transient solution for stress/strain

Under the assumptions described above, the displacements adjacent to a TS are purely radial, with the displacement field at distance r from the cavity center and shifted time τ given by [18]

$$u(r, \tau) = \frac{a^3 P}{4\mu r^2} \left[1 - \exp(-\zeta\tau) \left\{ \left(\frac{2r}{a} - 1 \right) \frac{\zeta}{\omega} \sin \omega\tau - \cos \omega\tau \right\} \right]$$

(EQ 2)

for $\tau > 0$ and $u(r, \tau) = 0$ for $\tau < 0$, where $\zeta = 2c_2^2/ac_1$, $\omega = \zeta\{(c_1^2/c_2^2) - 1\}^{1/2}$, and $\tau = t - \frac{r-a}{c_1}$. The longitudinal speed of sound is c_1 while the speed of sound of shear waves is denoted c_2 , where $c_1 = [(\lambda + 2\mu)/\rho]^{1/2}$ and $c_2 = [\mu/\rho]^{1/2}$. The shear modulus is μ and λ is Lamé's first parameter, $\lambda = K - 2\mu/3$, where K is the bulk modulus. The amplitude of the pressure pulse inside the cavity is denoted P_{max} and a is the radius of the pressurized spherical cavity. The shifted time τ equals zero when the stress pulse arrives at a material point at radius r .

In spherical coordinates, the radial (ϵ_{rr}) and tangential ($\epsilon_{\theta\theta} = \epsilon_{\phi\phi}$) strains are given by $\epsilon_{rr} = \frac{du}{dr}$ and $\epsilon_{\theta\theta} = \epsilon_{\phi\phi} = \frac{u}{r}$. Using the expression for $u(r, t)$, we obtain the following expressions for ϵ_{rr} and $\epsilon_{\theta\theta}$:

$$\epsilon_{\theta\theta} = \frac{a^3 P}{4\mu r^3} \left[1 + e^{-\zeta\tau} \left(\sin(\omega\tau) \frac{\zeta}{\omega} \left(1 - \frac{2r}{a} \right) + \cos(\omega\tau) \right) \right]$$

(EQ 3)

and

$$\epsilon_{rr} = -\frac{a^3 P}{4\mu r^3} \left[2 + e^{-\zeta\tau} \sin(\omega\tau) \left(\frac{\zeta^2(2r^2 - ar) - 2\zeta c_1(r-a) - ar\omega^2}{a\omega c_1} \right) + e^{-\zeta\tau} \cos(\omega\tau) \left(2 - \frac{2\zeta r^2}{ac_1} \right) \right]$$

(EQ 4)

The shear strain components are zero due to the purely radial displacement field. The isotropic, linear elastic constitutive relations yield the following radial σ_{rr} and tangential $\sigma_{\theta\theta} = \sigma_{\phi\phi}$ stresses: $\sigma_{rr} = (2\mu + \lambda)\epsilon_{rr} + 2\lambda\epsilon_{\theta\theta}$ and $\sigma_{\theta\theta} = \lambda\epsilon_{rr} + 2(\mu + \lambda)\epsilon_{\theta\theta}$. The shear stress components are zero because the shear strains are zero.

For the present work, we will assume that plastic flow initiates when the von Mises stress σ_{vM} exceeds a critical value. In terms of principal

stresses, $\sigma_{vM} = \sqrt{1/2(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_1 - \sigma_3)^2}$. For $\sigma_{rr} \neq 0$ and $\sigma_{\phi\phi} = \sigma_{\theta\theta} \neq 0$, $\sigma_{vM} = |\sigma_{rr} - \sigma_{\theta\theta}|$. Substituting the preceding expressions for stresses into this formula, we obtain σ_{vM} as a function of r and τ . We then determine the r and τ at which σ_{vM} reaches its maximum value. We find that σ_{vM} is maximum at $r = a$ and $\tau = 0$. It may be stated in simple analytical form:

$$\sigma_{vM}^{max} = \frac{2-\nu}{1-\nu} |P_{max}|.$$

(EQ 5)

This expression may be contrasted with one obtained for a spherical cavity with internal pressure P in static equilibrium with its surroundings:

$$\sigma_{vM}^{max}|_{equilibrium} = \frac{3}{2} |P|.$$

(EQ 6)

The factor $3/2$ in this expression is known as the stress concentration factor (SCF). By analogy, the factor $\frac{2-\nu}{1-\nu}$ in the expression for σ_{vM}^{max} may be termed the “dynamic” SCF. It is greater than the static SCF (by up to a factor of two) in the entire physically admissible range of Poisson’s ratios, $-1 < \nu < 0.5$.

The foregoing derivation of σ_{vM}^{max} considers only the rise in TS pressure to P_{max} and ignores its subsequent decay to near-vanishing levels as the liquid core of the TS cools. Our approach nevertheless provides an accurate expression for σ_{vM}^{max} because the maximum of σ_{vM} occurs at $r = a$ and $\tau = 0$. Thus, all subsequent reductions in TS pressure cause σ_{vM} in the surrounding material to decrease, but leave σ_{vM}^{max} unchanged. We have verified that the expression for σ_{vM}^{max} provided above is accurate by repeating our analysis for TS pressures that decay to zero after their initial rise to P_{max} (see section 4.3).

3.3 Maximum pressure inside thermal spikes

The rise in TS pressure to P_{max} occurs due to localized melting within the TS. Thus, we begin our calculation of P_{max} by finding the temperature rise inside the TS using the heat capacity per atom, $C_p = \frac{\Delta Q}{\Delta T}$, yielding

$$T_F = T_0 + \frac{\Delta Q}{C_p}.$$

(EQ 7)

Here, T_0 is the initial temperature, ΔQ is the average increase in energy per atom in the TS. As a first approximation, we evaluate T_F assuming a constant C_p equal to its value at the glass transition temperature, T_G .

We previously demonstrated that thermal spike energy deposition is due to the material-dependent nuclear stopping power S_n and is given by $\Delta Q = S_n L$, where L is the path length of the knock-on atom in the TS [17]. For approximately cylindrical TSs, with a radius r and length L , the energy deposited per TS unit volume is given by $\Delta Q/V_{TS} = S_n/(\pi r^2)$ [17]. For the as-quenched α -Cu_xNb_{1-x} alloys studied here, we previously found that a radius $r \approx 3.5$ nm yields values of energy per TS volume in good agreement with ones computed directly from atomistic modeling [17]. Determination of ΔQ in other alloys is addressed in the Discussion section.

If the material in the TS core were allowed to expand under zero external pressure, then the increase in temperature computed above would lead to a uniform thermal expansion.

$$\frac{\Delta V}{V_0} = 3\alpha_G(T_G - T_0) + 3\alpha_L(T_F - T_G).$$

(EQ 8)

The linear thermal expansion coefficient in the glass, α_G , is assumed to be constant up to T_G and the thermal expansion coefficient in the liquid, α_L , is taken as constant above T_G . This expression

applies to glasses that expand monotonically as temperature increases through T_G (as opposed to ones that contract upon melting [19]).

As shown previously [17], localized melting within TSs occurs in less than 1 ps and may therefore be viewed as instantaneous for the purpose of our analysis. Therefore, the liquid in a TS may be viewed as forming under constant volume, rather than constant pressure. To compute the pressure in the TS immediately after melting, we consider the compression of a liquid initially at zero pressure by a volumetric strain $-\frac{\Delta V}{V_0}$. The calculation uses the adiabatic compressibility, $\beta_S = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_S$. Taking the initial pressure to be zero and recognizing that $1/V$ is constant, we integrate β_S to obtain

$$P_f = \frac{1}{\beta_S} \frac{\Delta V}{V_0}.$$

(EQ 9)

As in the case of C_p , we evaluate β_S at T_G . Combining and simplifying all the foregoing expressions, we obtain:

$$P_f = \frac{3}{\beta_S} \left\{ \frac{\alpha_L S_n}{C_p \pi r^2} - (T_G - T_0)(\alpha_L - \alpha_G) \right\}$$

(EQ. 10)

3.4 TSIP figure of merit

Our TSIP figure of merit is obtained as the ratio of the maximum von Mises equivalent stress (σ_{vM}^{max}) to the material yield stress (σ_Y):

$$\chi = \frac{2-v}{1-v} |P_{max}| / \sigma_Y.$$

(EQ. 11)

Because the maximum pressure inside the TS is positive, we drop the absolute value. Using our expressions for P_{max} , we finally obtain:

$$\chi = \frac{3}{\beta_S} \left\{ \frac{\alpha_L S_n}{C_p \pi r^2} - (T_G - T_0)(\alpha_L - \alpha_G) \right\} \left(\frac{2-v}{1-v} \right) \frac{1}{\sigma_Y}$$

(EQ. 12)

4. Validation of TSIP figure of merit

To validate our FOM for TSIP, we conduct molecular dynamics simulations of 475 keV Nb PKAs in a -Cu_xNb_{1-x} amorphous alloys of three different compositions and two different processing histories (six simulations, in total). We identify thermal spikes (TSs) and find TS induced plasticity (TSIP) in adjacent unmelted material. We compare the maximum stress adjacent to TSs as well as maximum TS pressure to the predictions of the model developed in the previous section. Finally, we assess the predictive ability of the FOM in Eq. 12 against the amount of TSIP in the MD simulations.

4.1 Construction of atomic models

As in previous work [16, 17], we simulate 475 keV niobium (Nb) primary knock-on atoms (PKAs) passing through $\sim 1/2$ billion-atom models of an amorphous alloy of copper (Cu) and Nb (a -Cu_xNb_{1-x}). Our simulations use a classical embedded atom method (EAM) interatomic potential with Ziegler-Biersack-Littmark (ZBL) short-range interactions [20] in LAMMPS [21]. We construct models of a -Cu₂₅Nb₇₅ (500,000,000 atoms), a -Cu₅₀Nb₅₀ (474,353,318 atoms), and a -Cu₇₅Nb₂₅ (500,000,000 atoms) by quenching a 4,000 K liquid of the desired composition at 10^{13} K/s to 300 K in 25 K decrements under zero applied pressure. We use a velocity rescaling thermostat, a Nosé-Hoover NPH barostat, periodic boundary conditions, and a timestep size of $\Delta t = 2$ fs [22]. The three as-quenched models described above are further annealed at temperatures just below their glass transitions temperatures, T_G : 500 ps at 1500 K for a -

$\text{Cu}_{25}\text{Nb}_{75}$, 400 ps at 1200 K for $a\text{-Cu}_{50}\text{Nb}_{50}$, and 500 ps at 1250 K for $a\text{-Cu}_{75}\text{Nb}_{25}$. Thus, we generate a total of six models with two different preparation histories and three compositions.

To compute the physical properties of these models, we prepare smaller versions of amorphous $a\text{-Cu}_{25}\text{Nb}_{75}$ (48,668 atoms), $a\text{-Cu}_{50}\text{Nb}_{50}$ (48,778 atoms), and $a\text{-Cu}_{75}\text{Nb}_{25}$ (48,668) using the same quenching procedure as with the $\frac{1}{2}$ billion atom models. Sub- T_G annealed configurations are likewise prepared as described above. The structure and glass transition temperatures of these models have been previously reported [17, 23]. We determined T_G only in the as-quenched models and therefore assume in our analysis the same T_G for the annealed models. To enable evaluation of the FOM, χ , we determine the coefficients of thermal expansion, heat capacities, elastic constants, and yield stresses of these models. The results are given in Table 1.

The linear thermal expansion coefficient is computed from the 10^{13} K/s quench of the $\frac{1}{2}$ billion atom models as the first derivative of the cell length with respect to temperature, via the relation $\alpha_L(T) = \frac{1}{L} \frac{dL}{dT}$. Similarly, the constant-pressure heat capacity (C_P) was computed via the first derivative of enthalpy with respect to temperature: $C_P = \left(\frac{dH}{dT} \right)_P$ where $H = U + PV$. The quench is performed under zero pressure, so the PV term vanishes and only the total internal energy U contributes to the final value.

The elastic constants are computed under quasi-static loading at 0 K. Energy minimized structures are deformed with uniaxial tensile deformation in the z-direction in small strain increments ($\Delta\epsilon_{zz} = 10^{-5}$) and relaxed with steepest descent potential energy minimization after each strain increment. The models display linear elastic stress-strain response with $\sigma_{xx} = C_{12}\epsilon_{zz} + A$ and $\sigma_{zz} = C_{11}\epsilon_{zz} + B$. Since the models are elastically isotropic, we obtain $\mu = (C_{11} - C_{12})/2$, $\lambda = C_{12}$, and $\nu = \lambda/[2(\lambda + \mu)]$.

We compute the finite temperature yield stress using the 0.2% plastic strain offset criterion at 300 K using volume-conserving deformation with strain increments of $\Delta\epsilon_{vM} = 2 \cdot 10^{-4}$, each followed by molecular dynamics relaxation for $\Delta t = 0.1$ ps. Although the strain rate of these calculations ($\dot{\epsilon} = 2 \cdot 10^9$ 1/s) is high by the standards of conventional laboratory mechanical testing, it is in fact comparable to the strain rate imposed on material adjacent to TSs by the elastic pulse described in section 2 ($\dot{\epsilon} \approx 10^{10}$ 1/s).

The adiabatic liquid phase compressibility is the inverse of the bulk modulus (K), so we take $\beta_S = 1/K$. The bulk modulus of liquid Cu-Nb with the required composition is computed as the first derivative of pressure with respect to volume, $K = -VdP/dV$. It was obtained using isotropic volume contraction with strain increments of $\Delta\epsilon = 1 \cdot 10^{-3}$, each followed by finite temperature molecular dynamics relaxation for $\Delta t = 5$ ps.

4.2 Collision cascade simulations

We investigate the radiation response of both the as-quenched and annealed a -Cu-Nb models. During the collision cascade, NVE ensemble equations of motion are integrated using adaptive timesteps to ensure energy conservation. The simulation cell sizes are greater than the projected range of 475 keV Nb ions, computed using a version of SRIM [24] modified to exclude electronic stopping [25]. These simulations are described in detail in Ref. [17].

We analyze the MD collision cascade simulation results through reconstruction of atomic trajectories (“spaghetti analysis” [26]) and our previously reported voxel analysis method [16, 17]. We characterize local changes in physical quantities by computing their values in nano-scale cubic volumes (voxels). Voxel temperatures are computed by subtracting the voxel center of mass velocity from the voxel atom velocities and fitting the voxel atom kinetic energy distribution to the Maxwell-Boltzmann distribution [27], with temperature as the fitting

parameter [28]. Lagrangian voxel total strains are computed from the best-fit uniform deformation gradient between an initial ($t = 0$ ps) and final voxel atom configuration [29]. Plastic strains are computed by subtracting voxel elastic and thermal strains ϵ_{ij}^e from total strain, with $\epsilon_{ij}^e = S_{ijkl}\sigma_{kl} + \alpha\Delta T\delta_{ij}$, where σ_{kl} is voxel stress, S_{ijkl} is compliance tensor, α is thermal expansion, and ΔT is voxel temperature change. The system-specific elastic constants and thermal expansion coefficients were obtained in the smaller, ~ 50 k atom configurations, as described in the previous subsection (see Table 1).

In Fig. 2, we present the results of our collision cascade simulations. As illustrated in Fig. 2 (a-f), the single 475 keV Nb PKA (red trajectory) initiates numerous secondary knock-on atoms (SKAs – black trajectories) with a maximum kinetic energy $ke_{max} > 0.5$ keV that terminate in dense zones with numerous displacements between 0.5 and 1 nm (blue vectors). As previously discussed [17], the energy dissipation in sub-cascades yields localized melting in thermal spikes (TSs), as evidenced by the local temperature fields shown in Fig. 2 (g-l). In these simulations, the stress pulse generated by melting within TSs has sufficient intensity to induce permanent deformation. As shown in [16] (Figure S1), the stress pulse travels at the longitudinal speed of sound (~ 5000 m/s) and does not interact with its periodic images until times exceeding ~ 14.5 ps. To prevent periodic images of these stress pulses from interacting, we restart the simulation at 13.5 ps (before periodic image impingement) and equilibrate the system with Langevin 300 K thermostated adsorbing boundaries, which effectively damps the elastic pulses and enables analysis at later times (see [16, 17]). Fig. 2 (m-r) shows voxels whose tensile work equivalent plastic strains ϵ^p exceed 0.0125.

In all six simulations, we identify all voxels adjacent to all thermal spikes (i.e. ones where $350 \text{ K} < T_{max} < T_G$) and average their plastic strains tensors to obtain the average, system-

wide, irradiation-induced plastic strain tensor. We diagonalize this strain tensor to obtain its principal strains and directions. As shown in Fig. 3 (a), in each model, we find that one principal strain is negative, one is positive, and one is close to zero. The non-zero principal strains depend on composition and processing history.

We also investigate the alignment of the principal strain eigenvectors with the average cascade direction. The cascade direction is computed from the orientation of the major axis of the best-fit ellipsoid to the region where $T_{\max} > 350$ K. Alignment angles θ are computed as projections of strain eigenvectors onto the cascade direction. In all cases, we find that the eigenvector best aligned with the cascade direction is the one with the negative eigenvalue. We term the principal strain associated with this eigenvector as ϵ_{casc} . As may be seen in Fig. 3(b), with the exception of the annealed a -Cu₂₅Nb₇₅ and quenched a -Cu₇₅Nb₂₅ models, the alignment is very close, with $\theta < 20^\circ$. The other two eigenvectors (corresponding to eigenvalues that are positive and near zero) are therefore approximately perpendicular to the average cascade direction.

Thus, we expect that an amorphous metal alloy exposed to a unidirectional beam of particles will undergo a spontaneous compressive shape change in the direction of the beam. Within the plane normal to the average cascade direction, there is no preferred orientation for the eigenvalues corresponding to positive and near-zero principal strains. Thus, the average effect of numerous cascades will be to cause isotropic expansion in the plane perpendicular to the beam direction. Estimates of the TSIP-induced strain per unit fluence expected based on our simulations are given in Ref [16].

4.3 Validation of stress pulse model

To validate our model of the elastic stress pulse emitted by TSs (section 3.2), we compare its predictions with one of the TSs in our MD simulations. We focus on the TS boxed in Fig. 2 (o) and shown close-up in Fig. 4 (a). The TS may be approximated as a prolate ellipsoid with major axis 19.6 nm long and minor axes 5 and 3.3 nm in length. We model the TS with a sphere of equivalent volume, yielding a radius of $a = 4$ nm, which is close to the average of the two minor directions (4.1 nm).

In Fig. 4 (b), we plot the time-dependent pressure in the TS, averaged over all TS voxels. Within 0.3 – 0.5 ps, the pressure increases from $P \approx 0$ to $P \approx 15$ GPa and subsequently decreases to an equilibrium residual pressure of ~ 1 GPa after ~ 3 ps. The micromechanical model described in section 3.2 models TS pressure as a step function with pressurization of $P = 15$ GPa and does not capture the drop in TS pressure after ~ 3 ps. Therefore, in addition to the original “step model,” we also calculate the predictions of a “pulse model,” where the pressure rises rapidly and then drops, as shown in Fig. 4 (b). In this model, we superimpose the transient elastic solutions due to two step-function loadings: a positive step-function with pressurization of $P = 15$ GPa at $t = 0.5$ ps followed by a step-function with $P = -14$ GPa at $t = 1.0$ ps.

We evaluate the time-dependent von Mises stress at a radial distance of $r = 7$ nm (3 nm from the cavity surface) using both the step and pulse models. Material constants μ , λ , and ρ are those provided for α -Cu₅₀Nb₅₀ in Table 1. In Fig. 4(c), we plot predicted von Mises stresses along with the von Mises stress found adjacent to the TS in MD (average distance of 3.2 nm from TS surface). The timescale for the initial rise and decay of von Mises stress predicted by both the step and pulse models is in good agreement with the MD data. As expected, the long-time behavior of both models is very different: in the step model, the von Mises stress adjacent to the TS remains high at long times while in the pulse model it gradually decays to 1 GPa.

However, both models exhibit identical peak stresses. Since our FOM is based on the peak von Mises stress adjacent to TSs, the simpler step model is adequate for our purposes.

The predicted peak von Mises stress for both the step and pulse model is ~ 2 GPa higher than that found in MD. This is to be expected since both models are purely linear elastic and do not take into account stress relaxation through plastic deformation. By contrast, in the MD simulations, we expect that the von Mises stress adjacent to TSs does not exceed the yield stress due to onset of plastic flow. Indeed, Table 1 shows that the yield stress in α -Cu₅₀Nb₅₀ is ~ 3 GPa, in excellent agreement with the peak stress from MD simulations shown in Fig. 4 (c). Plastic flow also gives rise to residual elastic back-stresses, which may account for the slower decay of von Mises stress in the MD data than in the purely elastic pulse model prediction. Other potential sources of discrepancies between the linear elastic model and the MD simulations are our approximation of TSs as spheres and our neglect of interactions with other adjacent TSs. However, the elastic model and the MD exhibit reasonable overall agreement, validating the use of the former as a means to predicting TSIP.

As an additional test for the validity of our micromechanical model, we use the pulse model to compute the transient stress response $\sigma_{rr}(r, t)$ and $\sigma_{\theta\theta}(r, t)$ at each material point adjacent to the thermal spike and obtain the maximum $\sigma_{vM}(r, t)$ at each point. Using the von Mises yield criterion (i.e., yielding for $\sigma_{vM} > \sigma_Y$), we predict the spatial extent of plastic flow adjacent to TSs [Fig. 5 (a)]. For comparison, in Fig. 5 (b) we plot the binned average of the tensile work equivalent plastic strain as a function of distance from the surface of the TS analyzed in Fig. 4. We find that the length-scale of predicted plastically deformed region [Fig. 5 (a)] is in excellent agreement with the decay length of the plastic strain measured in MD [Fig. 5 (b)], further confirming that the micromechanical model captures the essential physics of TSIP.

4.4 Validation of pressure prediction

We validate the thermodynamic model for TS pressure described in section 3.3 by comparing its predictions with the pressure found in our MD simulations. For each individual TS in the MD simulations, we compute the average pressure as a function of time and find the maximum pressure. The average pressure for each system is then obtained as the average over the individual maximum TS pressures. The corresponding average temperature is found from TS temperatures at the time of the maximum pressure.

We test the pressure prediction for all six alloys using the micromechanical model for TS pressure. We evaluate TS pressure using Eq. 10 using material constants α , T_G , C_p , and β_S (computed as inverse of bulk modulus, K) obtained from independent equilibrium MD simulations. We compute the characteristic TS volume per unit deposited energy using the nuclear stopping model [17]. The values of all model parameters are given in Table 1.

We present the calculated pressures in Fig. 6, where we plot the TS pressure found in MD versus the pressure predicted from the micromechanical model. The order of magnitude of both quantities is in good agreement, i.e. all predicted thermal spike pressures fall between 10 and 18 GPa. Moreover, the micromechanical model captures the trend of increasing TS pressure with increasing copper concentration. However, we find that the micromechanical model under-predicts the TS pressure in α -Cu₂₅Nb₇₅ by ~20 % and over-predicts the pressure in α -Cu₇₅Nb₂₅ by ~10 %.

Thus, our micromechanical model is in qualitative agreement with the MD simulations. To identify the origin of quantitative discrepancies between them, we illustrate the calculation of the maximum TS pressure in Table 2, using physical parameters for a 475 keV Nb PKA irradiated as-quenched α -Cu₂₅Nb₇₅. From the average TS energy per atom and material heat

capacity, we predict TS temperature to be 3135 K, compared to the average TS temperature of 1816 K found from MD. We find similar differences in the $\text{Cu}_{50}\text{Nb}_{50}$ (3192 K predicted versus 1824 K simulated) and $\text{Cu}_{75}\text{Nb}_{25}$ systems (3225 K predicted versus 1940 K simulated).

We predict a volumetric expansion of 0.086, double the volumetric thermal expansion in a uniform $a\text{-Cu}_{25}\text{Nb}_{75}$ liquid at the measured average thermal spike temperature of 1825 K (0.044), with similar over-estimates in $a\text{-Cu}_{50}\text{Nb}_{50}$ and $a\text{-Cu}_{75}\text{Nb}_{25}$. To obtain the final pressure in the thermal spike, we multiply the predicted volumetric expansion by the bulk modulus at the glass transition temperature. In as-quenched $a\text{-Cu}_{25}\text{Nb}_{75}$, we predict 10.5 GPa, in comparison to the average TS pressure of 13.25 GPa. However, we under-predict TS pressure when we evaluate our model using the actual average TS temperature (1816 K), obtaining a predicted maximum TS pressure of 4.3 GPa. When our pressure prediction expression is evaluated in the other systems using the actual TS average temperature at the time of maximum TS pressure, we do find the correct trends but obtain a similarly large under-prediction of TS pressure.

Thus, we find that the relatively good agreement between the model predictions of pressure and the actual pressures found in the MD simulations is the outcome of over-prediction of the average TS temperature at the time of maximum TS pressure, in concert with an under-prediction of TS expansion. While this “cancelation of errors” is robust for predicting trends in this particular alloy system, it may prevent a systematic comparison between different compositions. In the discussion, we propose approaches to remedy these shortcomings for TS pressure prediction.

4.5 Validation of FOM by comparison with TSIP in MD simulations

As a final test for the model, we evaluate the FOM (Eq. 12) and compare the predicted susceptibility to TSIP (based on the FOM) with the actual TSIP found in the six 475 keV MD

simulations. As may be seen in Fig. 2, we find extensive plastic deformation adjacent to TS in all six MD simulations. Fig. 3(a) demonstrates that TSIP occurs in all simulations, including polarization of strains with respect to the overall cascade direction [Fig. 3 (b)].

Fig. 7(a) plots χ as a function of composition using the material parameters in Table 1. We find that χ varies by more than a factor of two over the range of investigated alloy compositions. To test how χ correlates with the extent of TSIP, we use the strain per unit fluence $A = f \times \epsilon_{casc}/\phi$: a parameter that is, in principle, experimentally measurable [16]. Here, f is the volume fraction of material that undergoes TSIP, ϕ is the specific fluence of the simulation (defined as the inverse of the model surface area, SA: $\phi = 1 \text{ PKA/SA}$), and ϵ_{casc} is the eigenstrain that is best aligned with the cascade direction (see section 4.2). Fig. 7(b) plots A as a function of the FOM. These two quantities are approximately linearly related for the as-quenched and annealed models.

Extrapolating the linear fit for A as a function of the FOM (χ) we find that $A = 0$ when $\chi = 1$, i.e. stress-pulse driven yielding ceases when the stress pulse amplitude falls below the system yield stress. This provides strong support for the fundamental hypothesis of our work: plastic deformation is driven by the TS-induced pressure pulse and proportional to the ratio of the stress-pulse magnitude to the system-specific yield strength.

5. Discussion

5.1 Opportunities for model improvement

The model we introduced for TSIP captures the mechanism observed in atomistic simulations, specifically:

- The model reproduces the time scale and magnitude of the stress pulse propagation from pressurized thermal spikes

- The model predicts the MD-based length-scale of plastic flow adjacent to TSs
- The model-based FOM reproduces the MD-based trends of composition-dependent magnitude of TSIP, including extrapolating to a TSIP of zero at a FOM of one.

The current model provides an accurate prediction of TS pressure, leading to reliable FOM predictions. However, as demonstrated in Section 4.4, the TS pressure prediction benefits from an effective cancelation of errors in the prediction of the maximum TS pressure through an over-prediction of TS temperature and an under-estimate of thermal expansion at a given temperature. Thus, while all aspects of the transient solid mechanics model are reliable, there is a need to improve the prediction of the TS pressure.

First, we suggest that if melting continues after the initial energy deposition due to heat conduction (e.g. in coalescence of adjacent TSs, see [17]), our model for isolated TSs with adjacent plastic deformation is no longer applicable. Supporting the potential complications that may arise from TS coalescence, we find a wide distribution of TS temperatures at the time of maximum TS pressure, including temperatures below the glass transition temperature. However, we previously found that TS coalescence is minimal for all of the as-quenched models, as well as annealed α -Cu₂₅Nb₇₅ [17].

Second, we hypothesize that high momentum recoils, generated during initiation of TSs, may increase TS pressurization above that expected from equilibrium melting and thermal expansion. Calder *et al.* observed stress pulse propagation in irradiated BCC iron to initiate with a supersonic shock front over the formative times of the cascade, ~ 0.1 ps, before transitioning to a sonic wave at later times, ~ 1 ps [26]. Such supersonic shock fronts at short times may increase the pressure in the TS above that expected from constrained liquid melting.

5.2 Evaluation of FOM in other amorphous metal alloys

Both the extent of TSIP (measured by parameter A) and χ vary by a factor of approximately two among the six atomic models used in our MD simulations [see Fig. 7 (b)]. This finding suggests that there may be a wide range of susceptibilities to TSIP among amorphous metal alloys in general, including in metallic glasses. It is possible that some might not exhibit TSIP at all, if their yield strength is higher than the von Mises stress generated by stress pulses emitted from TSs. Such wide variability in TSIP motivates an exploration of amorphous metal compositions to optimize radiation response. We therefore discuss how our FOM may be evaluated in other alloy systems, beyond the a-Cu-Nb investigated here.

As we initially proposed in Section 3.4, the FOM is given by the ratio of the maximum stress adjacent to TSs divided by the material yield strength, $\chi = \sigma_{vM}^{max}/\sigma_Y$, or $\chi = \frac{2-\nu}{1-\nu}|P_{max}|/\sigma_Y$. Fundamentally, this proposed FOM requires knowledge of the material yield stress σ_Y (preferably measured at high strain rates), Poisson ratio ν , and maximum TS pressure P_{max} . A unique feature of the physical mechanism of TSIP is that the high strain rates accessible in conventional MD simulations are directly comparable to the strain rates due to stress pulses adjacent to TSs. Therefore, the elastic constants and yield stress needed to compute the FOM may be conveniently obtained through standard MD simulations, as well as through experiments.

In Eq. 10, we proposed that P_{max} could be predicted using a thermodynamic model. In the model, we require knowledge of the following material properties: liquid phase isentropic compressibility β_S , thermal expansion α of both the glass and the liquid, glass transition temperature T_G , heat capacity C_p at the glass transition, and average energy per atom deposited in thermal spikes ΔQ . With the exception of ΔQ , all values may be obtained from MD simulations of quenching from the liquid. For some compositions, such simulations may be conducted using relatively small models containing ~ 100 atoms or fewer. If the required interatomic potentials are

available or if sufficiently large first principles simulations may be performed, then the calculation of these parameters may be automated for high-throughput screening of metallic glass compositions.

To predict the average TS temperature and the corresponding volumetric thermal expansion, our model uses the characteristic energy per TS, ΔQ , in the form of a nuclear stopping model for energy deposition in TSs: $\Delta Q/V_{TS} = S_n/(\pi r^2)$ (Section 3.3). By first calculating the nuclear stopping power using the binary collision cascade code SRIM, we found the radius r which yielded the best fit to the average energy flow into thermal spikes in our large-scale MD simulations [17]. Since TS size is a critical parameter of our nuclear stopping model, we propose that, in lieu of large-scale MD simulations, the most computationally efficient means to obtain ΔQ is through the continuum simulation strategy originally developed by Caro for crystalline materials [30, 31] and recently presented by Myers *et al.* for metallic glasses [32, 33]. These authors used the binary collision cascade code SRIM to generate positions of recoils and used the result to determine the transient temperature profile in 3D finite difference [30, 31] and finite element simulations [32, 33]. The spatial and temporal distribution of temperature they predicted is similar to the results we show in Fig. 2. TSs may then be identified via temperature isocontours $T = T_G$, as we have demonstrated through our voxel analysis of the MD simulations. Since the prediction the average TS temperature is the objective of our nuclear stopping model, this temperature can be used directly in our FOM expression in Eq. 10. The SRIM output also provides the TS energy density, which may be used to either evaluate ΔQ directly or to fit to a nuclear stopping model, such as the one we use in the FOM expression in Eq. 10.

However, as we discuss in Section 5.1, the current thermodynamic model for pressure does require improvement. Therefore, prediction of TS pressure across many different types of

alloys may require an approach altogether different from Eq. 10 to obtain quantitative predictions of melt-induced pressurization of thermal spikes. One approach could be direct MD simulation of confined melting. Once the average expected TS temperature is known, using the SRIM/continuum modeling strategy outlined above, a model of an amorphous material may be superheated to the average expected TS temperature using NVT MD, yielding a direct measure of the pressure associated with confined melting. This pressure may then be used to evaluate the complete FOM, in conjunction with measured or calculated material yield stress and elastic constants.

In the absence of simulation-based predictions or experimental measurements of physical properties, we propose that materials may be screened for susceptibility to TSIP on the basis of a few key physical properties. First, we propose that materials that minimize the ratio of the dynamic SCF, $\frac{2-\nu}{1-\nu}$, and the yield stress,

$$\Gamma = \left(\frac{2-\nu}{1-\nu} \right) / \sigma_Y$$

(EQ. 13)

will have greatest resistance to TSIP. Next, we propose that material glass transition temperature, T_G , will be inversely correlated with TS pressure. For a given characteristic TS temperature, materials with higher T_G will likely have lower thermal expansion (and thus TS pressure), since thermal expansion ought to depend on the TS temperature relative to its glass transition temperature. Therefore, materials with high T_G and low Γ will minimize TSIP. Johnson and Samwer collected mechanical properties—including Poisson ratio, yield stress, and glass transition temperature—for ~30 vitreous alloys [34]. We used their data to calculate Γ and plot it against T_G in Fig. 8 (see Table S1 for details). We find that there are indeed materials that have high T_G and low Γ and observe that our numerical results follow the expected trend of high T_G

and low Γ minimizing TSIP. Therefore, it would be of interest to probe some of the high T_G /low Γ materials, such as the alloys indicated in the legend of Figure 8.

5.3 Impact of PKA energy on TSIP

As we previously reported, we find a linear relationship between TS energy and volume, with a material-specific TS energy per unit volume (see Figure 9 in [17]). We therefore expect the TSIP mechanism to hold for KA energies exceeding the threshold energy for TS formation, i.e. ~ 0.5 keV. Below this energy, Mayr *et al.* suggest that, radiation-induced “point defects,” similar to the flow defects proposed by Spaepen within the free-volume theory for homogeneous flow [35, 36], can mediate viscous flow in stressed amorphous solids [37]. However, it is not clear whether these proposed structural defects induce plasticity under stress-free conditions. Xiao *et al.* suggest that low energy (e.g. ~ 100 eV) KAs do induce structural changes, leading to the formation of high fictive temperature material [38], but they do not report any radiation-induced plasticity. It would be interesting to investigate whether radiation-induced plasticity can occur in the absence of TSs, but such an investigation is beyond the scope of the current work.

5.4 Comparison of the TSIP model to ion-induced plasticity

Klaumünzer’s early work demonstrated a remarkable property of amorphous materials: anisotropic plastic deformation when bombarded by swift, heavy ions with kinetic energies in the electronic stopping regime [13, 39, 40]. Numerous studies have demonstrated that this ion-induced plasticity phenomenon in amorphous materials occurs in both metals [13, 41] and insulators [42].

However, the TSIP mechanism we describe and model here is qualitative different from the ion hammer effect. Beyond the difference in energy stopping regime (nuclear versus electronic stopping), the proposed mechanisms are different. Early work on ion-induced

plasticity proposed a “Coulomb explosion” whereby ionization of atoms in the path of the projectile leads to a positive repulsive force that drives expansion perpendicular to the ion’s path on a timescale much less than 1 ps [13, 39]. More recently, Trinkaus and Ryazanov [43] and later van Dillen *et al.* [44] suggested instead that plasticity occurs through relaxation of shear strains *inside* a viscous cylindrical region left by the penetrating ion. By contrast, here we have proposed that TSIP is the result of stress-pulse induced yielding *outside* of the TS, due to the dynamic stress-concentration induced by rapid pressurization of the TS from localized melting.

5.5 Why does TSIP not occur in crystalline alloys?

Thermal spikes are well known to occur in crystalline materials [45, 46]. Thus, it would appear that TSIP is, in principle, also possible in crystalline metals. Nevertheless, no experimental evidence for TSIP in crystalline metals is available. If it were to occur, TSIP in crystalline metals would involve the punching out of prismatic dislocation loops from TSs. Wolfer found that when the internal pressure in a circular cavity is about 20% of the shear modulus of the surrounding crystal [47], there is a thermodynamic driving force to emit such a loop. In crystalline Cu, 20% of the shear modulus is approximately 15 GPa, placing it within the range of TS pressures found in the present Article. However, while recent MD simulations report small interstitial clusters induced by stress pulses emitted from TSs [26, 48, 49], punching out of larger prismatic dislocation loops from TSs has so far not been observed [50]. We suggest two possible reasons to explain the apparent lack of TSIP in crystalline metals.

First, Wolfer’s estimate is based on calculations of thermodynamic driving forces and does not take into account the critical stress required to nucleate prismatic loops adjacent to a pressurized cavity [47]. This stress may approach the theoretical shear strength of a material, in some cases [51]. In our calculations, the maximum von Mises stress adjacent to a TS with 15

GPa internal pressure is about 5 GPa. This value—while high—falls short of the theoretical shear resistance of crystalline metals. By contrast, the theoretical shear strength of a metallic glass is likely to be close to its bulk flow resistance, i.e. much lower than the ideal shear strength of a single crystal. Thus, TSIP may be easier to initiate in metallic glasses than in crystalline metals.

Second, when a TS cools down, its internal pressure decreases (to approximately zero in crystalline metals), removing the driving force for dislocation loop emission. Elastic back-stresses may then drive previously generated loops—which glide easily—back into the TS core, reversing the plastic deformation. Thus, even if TSIP were to occur in crystalline materials, it is likely to be a local, transient, and reversible phenomenon. By contrast, plastic deformation in amorphous alloys is much more difficult to reverse: it would entail re-initiating reverse plastic flow at stresses comparable to those needed to cause plastic flow in the initial (forward) direction. Consequently, local TSIP in amorphous materials is not expected to be fully reversible. Rather, TSIP contributions from multiple TS accumulate, eventually giving rise to a macro-scale shape change. TSIP therefore appears to be distinctive of amorphous materials.

6. Conclusions

We use continuum linear elasticity and thermodynamics to develop a model that predicts the susceptibility of metallic glasses to thermal spike induced plasticity (TSIP). Using this model, we formulate a figure of merit (FOM) to rank the relative susceptibilities of different metallic glasses to TSIP. The FOM is defined as the ratio of the maximum von Mises stress generated by stress pulses emitted from thermal spikes (TSs) to the yield stress of the material: $\chi = \sigma_{vM}^{max} / \sigma_Y$. We validate our FOM by comparing it with molecular dynamics (MD) simulations of TSIP in six amorphous Cu-Nb models of differing composition and processing

history. This comparison shows that χ is indeed able to rank the relative susceptibility of the a - $\text{Cu}_x\text{Nb}_{1-x}$ amorphous metal alloys to TSIP. However, application of the FOM for quantitative ranking of the relative susceptibility of other alloys to TSIP may require refinements of our thermodynamic model for the maximum pressure in thermal spikes. Therefore, we suggest that material yield stress, Poisson ratio, and glass transition temperature may be sufficient for screening of candidate alloys for susceptibility to TSIP, and we utilize previously reported material properties to identify candidate alloy compositions for further investigation.

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Table Captions:

Table I: Table 1: Properties of amorphous Cu-Nb models calculated from molecular dynamics simulations. *Calculated using the nuclear stopping model with $r = 3.5$ nm [17].

Table II: Calculation of maximum TSs pressure based on the model in Section 3.3 using the data in Table 1. $^*\Delta V/V_0(T_F = 3200\text{ K}) = 0.13$; $\Delta V/V_0(T_F = 1825\text{ K}) = 0.044$.

Figure Captions:

Fig. 1: Illustration of the mechanism of thermal spike induced plasticity (TSIP). (a) Energy deposition via nuclear stopping; (b) localized melting leading to the formation of a thermal spike (TS); (c) pressurization of the TS due to thermal expansion of the liquid in its core; (d) plastic deformation from high intensity stress pulse; (e) rapid quenching to amorphous, high fictive temperature super-quenched zone (SQZ).

Fig. 2: MD simulations of 475 keV Nb PKA collision cascades in $a\text{-Cu}_{25}\text{Nb}_{75}$, $a\text{-Cu}_{50}\text{Nb}_{50}$, and $a\text{-Cu}_{75}\text{Nb}_{25}$ amorphous alloys in both their as-quenched and annealed states. Radiation-induced displacements are shown in the left-hand column (a-f); TSs with $T_{max} > T_G$ (red voxels) and a region heated $T=350\text{ K}$ (blue contour) shown in the center column (g-l); and voxels exhibiting TS-induced plasticity (TSIP) with $\epsilon^p > 1.25\%$ are shown in black in the right-hand column (m-r).

Fig. 3: (a) Principal components of the average plastic strain in the models shown in Fig. 2 (the uncertainty of the mean is smaller than the symbols). Here, ϵ_{casc} is the principal strain whose eigenvector is best aligned with the average cascade direction and ϵ_{l1} and ϵ_{l2} are the two lateral principal strains orthogonal to the cascade direction. (b) Alignment between the cascade direction and the eigenvector of ϵ_{casc} .

Fig. 4: (a) Approximation of the TS boxed in Fig. 2(o) as a sphere with radius $a=4$ nm. Black cubes are voxels with plastic strain $\epsilon_{VM}^p > 1.25\%$. (b) Comparison of MD TS pressure (blue line with symbols) with step and pulse model pressurization profiles (dashed and solid lines, respectively). (c) von Mises stress adjacent to the TS from MD (blue line with symbols) compared with micromechanical model predictions based on step and pulse pressurization (dashed and solid lines, respectively).

Fig. 5: (a) Prediction of maximum von Mises stress (σ_{VM}) as a function of distance from the surface of a spherical TS. (b) Average tensile work equivalent plastic strain as function of distance from surface of the TS boxed in Fig. 2(o) and shown in Fig. 4(a). Errorbars indicate uncertainty on the mean.

Fig. 6: Average TS pressure in MD simulations of as-quenched (closed symbols) and annealed (open symbols) α -Cu-Nb models plotted against pressure predicted by the model in Section 4.4. Error bars indicate uncertainty on the mean.

Fig. 7: (a) Variation of χ , evaluated using the proposed micromechanical model, with material composition. (b) Variation of average TSIP plastic strain versus calculated FOM, χ . The solid vertical line at $\chi = 1$ indicates the FOM value below which no TSIP is expected to occur. The legends in (a) and (b) apply to both figures.

Fig. 8: Glass transition temperature (T_G) versus simplified TSIP predictor, Γ . Filled symbols: as-quenched material properties for the three Cu-Nb alloys reported here. Empty symbols: alloy properties reported in [34].

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Fig. 2: MD simulations of 475 keV Nb PKA collision cascades in $a\text{-Cu}_{25}\text{Nb}_{75}$, $a\text{-Cu}_{50}\text{Nb}_{50}$, and $a\text{-Cu}_{75}\text{Nb}_{25}$ amorphous alloys in both their as-quenched and annealed states. Radiation-induced displacements are shown in the left-hand column (a-f); TSs with $T_{\max} > T_G$ (red voxels) and a region heated $T=350$ K (blue contour) shown in the center column (g-l); and voxels exhibiting TS-induced plasticity (TSIP) with $\epsilon^p > 1.25\%$ are shown in black in the right-hand column (m-r).

Fig. 3: (a) Principal components of the average plastic strain in the models shown in Fig. 2 (the uncertainty of the mean is smaller than the symbols). Here, ϵ_{casc} is the principal strain whose eigenvector is best aligned with the average cascade direction and ϵ_{l1} and ϵ_{l2} are the two lateral principal strains orthogonal to the cascade direction. (b) Alignment between the cascade direction and the eigenvector of ϵ_{casc} .

Fig. 4: (a) Approximation of the TS boxed in Fig. 2(o) as a sphere with radius $a=4$ nm. Black cubes are voxels with plastic strain $\epsilon_{VM}^p > 1.25\%$. (b) Comparison of MD TS pressure (blue line with symbols) with step and pulse model pressurization profiles (dashed and solid lines, respectively). (c) von Mises stress adjacent to the TS from MD (blue line with symbols) compared with micromechanical model predictions based on step and pulse pressurization (dashed and solid lines, respectively).

Fig. 5: (a) Prediction of maximum von Mises stress (σ_{vM}) as a function of distance from the surface of a spherical TS. (b) Average tensile work equivalent plastic strain as function of distance from surface of the TS boxed in Fig. 2(o) and shown in Fig. 4(a). Errorbars indicate uncertainty on the mean.

Fig. 6: Average TS pressure in MD simulations of as-quenched (closed symbols) and annealed (open symbols) $a\text{-Cu-Nb}$ models plotted against pressure predicted by the model in Section 4.4. Error bars indicate uncertainty on the mean.

Fig. 7: (a) Variation of χ , evaluated using the proposed micromechanical model, with material composition. (b) Variation of average TSIP plastic strain versus calculated FOM, χ . The solid vertical line at $\chi = 1$ indicates the FOM value below which no TSIP is expected to occur. The legends in (a) and (b) apply to both figures.

Fig. 8: Glass transition temperature (T_G) versus simplified TSIP predictor, Γ . Filled symbols: as-quenched material properties for the three Cu-Nb alloys reported here. Empty symbols: alloy properties reported in [34].

Tables

Temp	Properties	Quenched <i>a</i> -Cu ₂₅ Nb ₇₅	Annealed <i>a</i> -Cu ₂₅ Nb ₇₅	Quenched <i>a</i> -Cu ₅₀ Nb ₅₀	Annealed <i>a</i> -Cu ₅₀ Nb ₅₀	Quenched <i>a</i> -Cu ₇₅ Nb ₂₅	Annealed <i>a</i> -Cu ₇₅ Nb ₂₅
T_G	T_G [K]	1600	N/A	1500	N/A	1400	N/A
	$\beta_s(T_G) \sim 1/K$ [GPa ⁻¹]	8.18×10^{-3}		8.70×10^{-3}		9.78×10^{-3}	
	C_p [eV/(atom K)]	3.73×10^{-4}		3.63×10^{-4}		3.70×10^{-4}	
	$\alpha_L(T_G)$ [10^{-6} 1/K]	12.8		17.3		23.9	
300 K	α_G [10^{-6} 1/K]	6.9		8.9		12.2	
	σ_Y [GPa]	3.51	3.31	2.97	3.05	2.37	2.51
	ρ [g cm ⁻³]	8.2347	8.2415	8.1958	8.2039	8.2337	8.2387
	$S_n/\pi r^2$ [nm ³ /keV]*	15.9		14.9		13.7	
0 K	μ [GPa]	49.0 ± 0.1	50.0 ± 0.1	48.3 ± 0.1	48.6 ± 0.2	41.2 ± 0.2	42.6 ± 0.1
	λ [GPa]	131.3 ± 0.04	131.4 ± 0.06	130.8 ± 0.03	131.5 ± 0.1	129.7 ± 0.1	130.1 ± 0.03

Table 1: Properties of amorphous Cu-Nb models calculated from molecular dynamics simulations. *Calculated using the nuclear stopping model with $r = 3.5$ nm [17].

Quantity of interest	Analytical expression	Physical parameters for MD simulation of 475 keV Nb ion in <i>a</i> -Cu ₂₅ Nb ₇₅	Predicted value	Simulated value/source
Thermal spike temperature	$T_F = T_0 + \frac{\Delta Q}{C_p}$	$T_0=300$ K, $\Delta Q = [S_n/\pi r^2]^{-1}/\rho=1.085$ eV/atom $C_p(T_G) = 3.73 \times 10^{-4}$ eV/(atom K)	3206 K	1816 ± 168 K
				Thermal spikes
Change in Volume	$\frac{\Delta V}{V_0} = \frac{3\alpha_G(T_G - T_0) + 3\alpha_L(T_F - T_G)}{3\alpha_G(T_G - T_0) + 3\alpha_L(T_F - T_G)}$	$\alpha_G(T_0) = 6.9 \times 10^{-6}$ 1/K $\alpha_L(T_0) = 12.8 \times 10^{-6}$ 1/K $T_0=300$ K, $T_G=1600$ K $T_F = 3206$ K (expression above)	0.088	0.044*
				Quenched liquid
Thermal spike pressure	$P_f = K \frac{\Delta V}{V_0}$	$K(T_G) = 122.2$ GPa $\frac{\Delta V}{V_0} = 0.088$ (expression above)	10.8 GPa	13.25 ± 0.35 GPa
				Thermal spikes

Table 2: Calculation of maximum TSs pressure based on the model in Section 3.3 using the data in Table 1. * $\Delta V/V_0(T_F = 3200$ K) = 0.13; $\Delta V/V_0(T_F = 1825$ K) = 0.044.