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Temperature dependent dislocation bypass mechanism for coherent precipitates in Cu-Co alloys

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Abstract

Molecular dynamics simulations of dislocation interaction with coherent cobalt precipitates embedded in Cu-Co alloys reveal a temperature dependent bypass mechanism. Below 300 K, the trailing partial dislocation clearly bypasses the coherent, face centered cubic (FCC) cobalt precipitate by Orowan looping, caused by a reversible structural transformation as the leading partial locally converts the precipitate to the lower-energy hexagonal close packed (HCP) structure. The FCC versus HCP energy difference of cobalt is temperature dependent, and the dislocation bypass mechanism becomes pure shear above 300 K. Based on a combination of inertial effects due to phonon drag and this observed bypass mechanism, we develop a temperature dependent critical resolved shear stress (CRSS) model, which is in excellent agreement with long-standing measurements of the CRSS temperature dependence of Cu-Co alloys, and those obtained from MD simulation. The model explains both the CRSS increase at low temperatures and the existence of a peak value around 200 K.

Keywords: Precipitation strengthening; Dislocation glide; Critical resolved shear stress; Molecular dynamics simulation; Cu-Co alloy

1. Introduction

Cu-Co alloys, which exhibit giant magnetoresistance (GMR) behavior as either multilayer thin films [1] or alloys with embedded cobalt nanoparticles [2], have been studied as a model precipitate-hardened alloy system since the 1950's [3-9]. Ferromagnetic cobalt has limited solubility in copper, and a relatively small lattice mismatch ($< 2\%$). Thus, cobalt precipitates rapidly form during thermal aging from super-saturated solutions and maintain a coherent, face-centered cubic (FCC) transition phase until losing coherency at larger sizes and transforming to the equilibrium hexagonal close-packed (HCP) structure. Transmission electron microscopy (TEM) studies of the shape, interfacial structure and ripening behavior of Co precipitates in Cu have shown that the FCC Co particles are roughly spherical and maintain interfacial coherency with a cube-cube orientation relationship until the precipitate size reaches about 10 nm [8].

Nembach and co-workers [10,11] studied the critical resolved shear stress (CRSS) of Cu-Co single crystals and discovered an anomalous temperature dependence. In their studies, coherent cobalt precipitates with a mean diameter of about 6 nm and estimated to contain 93% Co were formed by heat treating single crystal Cu-Co alloys containing up to 2.2 atomic percent cobalt [10,11]. Single crystals were compression tested from 12 to 500 K at a strain rate of $\sim 1 \times 10^{-4} \text{ s}^{-1}$. Fig. 1 shows the temperature dependence of the CRSS for pure Cu and alloys containing 0.93, 1.28 and 2.23% volume fraction of the cobalt precipitates, as reproduced from Fusenig and Nembach [11]. In the precipitate hardened alloys, the CRSS increases with temperature to a maximum value at a temperature around 170 to 230 K, and then decreases at higher temperatures. In these

1 alloys, the CRSS at 500 K is similar to that measured around 10 K. Notably, there is
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3 essentially no temperature dependence of the CRSS in the pure Cu single crystal [11].
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5 Büttner and Nembach [10], and later Fusenig and Nembach [11], attributed the low
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7 temperature behavior to dynamic dislocation effects resulting from inertia and phonon
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9 drag, which notably disappeared with the addition of increasing concentrations of Au to
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11 the Cu-Co alloys as a solid solution strengthener [11]. However, the observed CRSS was
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13 temperature independent for larger, presumably incoherent precipitates of 40 and 80 nm
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15 diameter over the range of 10 to 300 K [11]. At higher temperatures, it is generally
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17 assumed that thermally activated dislocation climb processes dominate and the material
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19 softens [12]. While these mechanisms partially explain the temperature dependence of the
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21 CRSS of precipitation hardened Cu-Co alloys; the entire temperature dependence and, in
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23 particular, the temperature of the maximum CRSS resolved shear stress at a relatively
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25 low value of about 200 K remain to be fully understood.

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27 Complete resolution of the temperature dependence of the CRSS requires detailed
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29 atomistic insight into the mechanisms of the dislocation - precipitate interaction. In this
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31 paper, we describe large-scale molecular dynamics (MD) simulations of the interaction
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33 between gliding dislocations, of edge or screw character, and 3 nm diameter coherent
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35 cobalt precipitates in copper over a temperature range of 10 to 400 K. These results
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37 inform a temperature dependent critical resolved shear stress (CRSS) model, based on a
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39 combination of inertial effects due to phonon drag and the observed dislocation bypass
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41 mechanism, which agrees well with the experimental observations.
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58 **2. Computational methods**

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The MD simulations were performed with a modified version of the MDCASK code [13], and used the embedded atom method (EAM) [14] potentials from Foiles *et al.* [15] and Pasianot and Savino [16] to describe the atomic interactions in pure Cu and Co, respectively. The Cu-Co interactions have been described using the cross pair potential constructed by Nordlund and Averback [17]. They optimized the term so that the potentials can reproduce experimental information such as heat of mixing, lattice parameter and decomposition behavior of Cu-Co alloys, which seems to be appropriate for the description of the interface between a Co precipitate and a Cu matrix. The calculated shear moduli and stacking fault energies of FCC Cu and FCC Co at 0 K are presented (Supplementary Table 1). With these potentials, the shear modulus of FCC Co is about two times larger than that of FCC Cu and the lattice parameter of FCC Co is about 2 % larger than FCC Cu. Therefore, modulus mismatch is expected to govern the dislocation - precipitate interaction in the MD simulations, opposite to the experiments where lattice coherency strains are proposed to dominate the dislocation – precipitate interaction [18]. Notably, the stacking fault energy of Co is negative, accurately reproducing the fact that the HCP Co phase is favored at low temperatures (Supplementary Fig. 1).

The simulation cell consists of an FCC lattice, bounded by $(\bar{1}11)$, (110) and $(1\bar{1}2)$ faces in $X = a[\bar{1}11]$, $Y = a/2[110]$ and $Z = a/2[1\bar{1}2]$ directions, respectively. The cell dimensions for the simulations of edge dislocations are approximately 31 x 38 x 27 nm (X , Y and Z directions), and contain about 2.7 million atoms; for the simulation of screw dislocations, the cell dimensions are approximately 31 x 26 x 66 nm (X , Y and Z directions), and contain about 4.5 million atoms. Periodic boundary conditions are

applied in the Y and Z directions. The X surface is initially free, but is subject to a constant surface traction following equilibration. The surface traction provides a shear stress to drive dislocation motion. A coherent FCC Co precipitate about 3 nm in diameter is inserted symmetrically across the dislocation glide plane, maintaining the cube-cube orientation relationship with the matrix. The precipitate is placed at the center of the cell in the X direction for both edge and screw dislocations. An edge dislocation with $\mathbf{b} = a/2[110](\bar{1}11)$ is introduced 13 nm below the precipitate in the Y direction by removing two (220) half planes. A screw dislocation is introduced at the center of the cell based on the continuum elastic displacement field solution for a screw dislocation, which is 16 nm away from the precipitate in the Z direction. For the edge dislocation, this cell corresponds to a dislocation density of about $8 \times 10^{14} \text{ m}^{-2}$, and a precipitate number density of $3 \times 10^{22} \text{ m}^{-3}$, with a periodic spacing of 27 nm along the dislocation line. For the screw dislocation, this cell corresponds to a dislocation density of about $5 \times 10^{14} \text{ m}^{-2}$, and a precipitate number density of $2 \times 10^{22} \text{ m}^{-3}$, with a periodic spacing of 26 nm along the dislocation line. The dislocations naturally dissociate into two Shockley partials with Burgers vectors $\mathbf{b}_1 = a/6[211](\bar{1}11)$ and $\mathbf{b}_2 = a/6[12\bar{1}](\bar{1}11)$ with a mean separation of about 7 and 4 nm for the edge and screw dislocations, respectively, due to the low stacking fault energy of Cu with this EAM potential [15].

Before applying a shear stress, the cell was equilibrated for 60 ps in the temperature range 10-400 K. No special static relaxation was performed to stabilize the atomic positions around the dislocation. A constant shear stress in the range of 50-100 MPa is applied by superimposing a constant (equal and opposite) force in the $[110]$ direction on the atoms in the outermost $(\bar{1}11)$ surfaces. During the application of the shear stress, the

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4 velocities of all atoms were re-scaled every 10 steps by multiplying the square root of the
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6 ratio of target temperature (average kinetic energy) to current temperature (average
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8 kinetic energy) to maintain constant temperature. While the atomic velocity distribution
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10 might not precisely follow the ensemble average with this velocity scaling method, the
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12 temperature fluctuation due to the application of the shear stress can be minimized. This
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14 is an important consideration given that the dislocation bypass mechanism at the
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16 precipitate can be very sensitive to temperature change. A time step of 1 fs is used
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18 throughout the simulation. The common neighbor analysis (CNA) [19,20] has been used
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20 to visualize the dislocation cores. CNA distinguishes close-packed atomic structures such
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22 as FCC, HCP and icosahedron from non-close-packed atomic structures by analyzing
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24 bond pairs. The dislocation cores have been visualized by selecting atoms with non-
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26 close-packing structures. Visualization of these MD snapshots has been performed using
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28 the AtomEye code [21].
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36 We have also developed a phenomenological model to describe the temperature
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38 dependence of the CRSS based on our observation of the strongly temperature dependent
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40 precipitate obstacle resistance from coherent cobalt precipitates in copper, resulting from
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42 this new dislocation bypass mechanism. To account for the inertial effects of phonon drag
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44 on dislocation motion, the model incorporates an effective stress contribution to the
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46 overall CRSS, based on assuming that the resistance to dislocation motion from the
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48 inertial effects of phonon drag can be described by the well-known relation between an
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50 effective drag stress and a friction coefficient [22]. Correspondingly, we use a root sum
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52 square superposition to define the overall temperature dependent CRSS by combining the
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effective phonon drag resistance stress with the dispersed obstacle strengthening, which captures the temperature dependence of these two different mechanisms.

3. Results and discussion

Fig. 2 shows snapshots from the MD simulation of edge dislocation interaction with a 3 nm Co precipitate at 300 K and an applied shear stress of 100 MPa. During equilibration, the 3 nm, FCC Co precipitate maintains coherency with the Cu matrix, without any indication of impending structural transformation or interface instability. The edge dislocation is noticeably split into two Shockley partials with a mean separation of about 7 nm, which glide in the Y direction. After about 16 ps of applied stress, the leading partial initially contacts the Co precipitate (Fig. 2a). By about 23 ps, the leading partial shears the precipitate, noticeably bowing with a critical angle of about 70° (Fig. 2b). As the leading partial moves past the particle, the trailing partial begins to interact with the precipitate (Fig. 2c). By about 44 ps, the leading partial has moved through the periodic boundary conditions and re-entered the cell from the bottom (Figs. 2c and d), while the trailing partial continues to be pinned by the precipitate. About 45 ps after the applied stress, the trailing partial dislocation bypasses the precipitate by the expected shear mechanism (Fig. 2e). Noticeably, the resistance due to the precipitate is stronger for the trailing rather than the leading partial, with a critical bypass angle of approximately 50° as the trailing partial detaches from the precipitate (Fig. 2e). Considering the atomic arrangement of the Co precipitate before and after during dislocation bypass, the two central atomic layers of the precipitate take an HCP stacking after the bypass of the leading partial, which indicates the precipitate lies on the stacking fault (Supplementary

Fig. 2). After the bypass of the trailing pass, these atomic layers return to an original FCC stacking out of the stacking fault, but with a sheared shape of the precipitate. A similar process occurs for the 2nd subsequent bypass of the leading and trailing partials. MD simulations at 400 K reveal a similar sequence of events and interaction/detachment mechanism, namely that both the leading and trailing Shockley partial dislocations bypass the coherent Co precipitate by the expected shear mechanism, with the trailing partial experiencing more resistance. For detailed MD simulation results, see Supplementary Movie 1.

Fig. 3 shows snapshots from the MD simulation at 100K. The results are similar to those at 300 K for the leading partial dislocation, but the bypass mechanism for the trailing partial is completely new and unexpected. After about 15 ps of applied stress, the leading partial initially contacts the Co precipitate (Fig. 3a). By about 22 ps, the leading partial shears the precipitate, noticeably bowing with a critical angle comparable to the higher temperature simulation (Fig. 3b). As the leading partial moves past the particle, the trailing partial begins to interact with the precipitate. By about 41 ps, the leading partial has moved through the periodic boundary conditions and re-entered the cell from the bottom (Figs. 3c and d), while the trailing partial continues to be pinned by the precipitate, bowing to a critical angle of nearly 0°. As the trailing partial nearly completely surrounds the precipitate (Figs. 3d and e), the partial dislocation dipole segments just beyond the precipitate strongly interact and annihilate. This releases the trailing partial dislocation from the precipitate and leaves an Orowan loop around the precipitate, with partial dislocation character (Fig. 3e). The resulting Orowan loop, with a Burgers vector of $\mathbf{b}_2 = a/6[12\bar{1}](\bar{1}11)$, does not have a perfectly symmetric circular shape,

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4 but rather is elliptical in which some segments penetrate the precipitate. This glide loop is
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6 not energetically stable at this size and collapses, resulting in the additional shear of the
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8 precipitate, as the trailing partial completely moves past the particle (Fig. 3f). Viewing
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10 the final precipitate configuration from an edge-on, $\langle 111 \rangle$ projection (although not
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12 shown here), reveals precipitate shear by a full Burgers vector, $\mathbf{b} = a/2[110](\bar{1}11)$, even
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14 though the trailing precipitate did not bypass by the anticipated shear mechanism. For
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16 details, see Supplementary Movie 2. The same bypass mechanism also occurs, and is
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18 somewhat easier to visualize, for a larger precipitate (Supplementary Movie 3).
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24 Each MD simulation of edge dislocation - Co precipitate interaction with an 100 MPa
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26 applied shear stress and temperatures between 10 and 200 K showed this bypass
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28 mechanism involving a mix of shear for the leading partial dislocation and Orowan
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30 looping of the trailing dislocation. The different dislocation bypass mechanism for the
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32 leading and trailing Shockley partial dislocations, manifested by a different critical
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34 bowing angle for each partial, clearly indicates that the Co precipitate offered more
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36 resistance to the trailing partial. Even though the resulting Shockley partial (Orowan)
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38 dislocation loop collapsed, producing the net result of a sheared precipitate by one perfect
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40 Burgers vector, its obstacle strength is clearly temperature dependent, with the precipitate
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42 being a stronger obstacle at low temperatures than a simple shearable particle.
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48 An important question to ask is whether this behavior is unique to the edge
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50 dislocation? Fig. 4 presents results from the interaction between a screw dislocation and
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52 the 3 nm coherent cobalt precipitate, at a temperature of 100K and an applied shear stress
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54 of 100 MPa. The screw dislocation also dissociates into two Shockley partials, but with a
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56 smaller mean separation of about 4 nm. By about 26 ps, while the leading partial shears
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the precipitate with a critical bowing angle of about 80° , the trailing partial initially contacts the precipitate (Fig. 4a). About 20 ps after the leading partial completely passed through the precipitate by shear, the trailing partial surrounds the precipitate until a critical bowing angle reaches almost 0° (Fig. 4b). Then, the trailing partial is detached from the precipitate, leaving an Orowan loop around the precipitate (Fig. 4c). Shortly after the trailing partial detaches via the Orowan mechanism, the resulting Orowan glide loop collapses into the precipitate, again resulting in the shear of the precipitate by a full Burgers vector (Fig. 4d). These snapshots indicate that the mixed shear and Orowan bypass mechanism is also true for screw dislocations. For details, see Supplementary Movies 4 and 5.

This new, mixed shear and Orowan dislocation bypass mechanism and the transition in mechanism with temperature observed in MD simulations can be understood by considering the precipitate resistance to dislocation motion. For shearable coherent precipitates, the resistance to dislocation motion results primarily from elastic modulus mismatch or difference in atomic size (or lattice parameter) between the precipitate and matrix, in addition to secondary contributions from interface generation [18,22]. None of these mechanisms should differ substantially for the two Shockley partial dislocations, nor have strong temperature dependence. For the specific case of coherent cobalt precipitates embedded in an FCC Cu matrix, a new strengthening mechanism must be considered, due to the reversible crystallographic structural transformation of the precipitate, which is different for each of the two Shockley partial dislocations.

As the leading partial shears the precipitate by $a/6[1\bar{2}1]$, a plane of HCP stacking (e.g., the FCC stacking fault which separates partial dislocations) is introduced within the

precipitate on the dislocation glide plane. As shown in Supplementary Table 1, HCP Co is energetically favored to FCC Co, and thus, additional work is required to transform the now HCP structure on the dislocation glide plane within the precipitate back to an FCC structure. This imparts resistance that acts against the trailing Shockley partial dislocation. The maximum force imparted on the trailing partial dislocation can be calculated as,

$$F_{\max} = \frac{\pi R^2 |\gamma_{\text{SFE}}|}{b} \quad (1)$$

where R is the precipitate radius, b is the dislocation Burgers vector and γ_{SFE} is the stacking fault energy, which defines the difference in energy between planar FCC and HCP stacking. Since HCP cobalt is energetically preferred at low temperatures, γ_{SFE} of the FCC phase is negative and the absolute value is introduced into Eq. (1). The CRSS on the dislocation due to the structural transformation force given by Eq. (1) is obtained from a conventional dispersed barrier hardening relationship [18],

$$\tau_{\text{CRSS}} = \frac{F_{\max}}{bL} \quad (2)$$

where L is the inter-particle spacing, which we take equal to the periodic spacing along the dislocation line less the precipitate diameter. Following Ashby [23], the critical stress for Orowan looping of an edge dislocation about an impenetrable obstacle is

$$\tau_{\text{CRSS}} = \frac{Gb}{2\pi} \frac{1}{L} \ln\left(\frac{x}{r_o}\right) \quad (3)$$

where G is the shear modulus, which for our simulation geometry is that of the shear modulus on the $\{111\}$ plane in the $\langle 110 \rangle$ direction, namely $(3C_{44}(C_{11}-C_{12}))/((C_{11}-C_{12}+4C_{44}))$ [24], x is the particle diameter and r_o represents the dislocation core radius, which we assume equals $\sqrt{2}b$.

The Gibbs free energy difference between HCP and FCC cobalt decreases linearly with increasing temperature until becoming zero at about 700 K [25]. Thus, we assume the same linear temperature dependence for the (negative) stacking fault energy, from the known value of -37 mJ/m² at 0 K (Supplementary Table 1) to 0 mJ/m² at 700 K. Fig. 5a plots the predicted CRSS, normalized to the maximum Orowan strength (Eq. 2, using elastic constants at 1K), due to precipitate strengthening obtained using equations (1) and (2) for a 3 nm diameter Co precipitate based on the (new) structural phase transformation precipitate strengthening mechanism (shown in black) and compares it to the Orowan strength obtained from Eq. (3) (shown in blue). In both calculations, we assume a temperature dependence of the copper elastic constants, consistent with the published values (Ref. 26). The resulting strengthening effect of the precipitate on dislocation motion should be the minimum CRSS between that given by Eqs. (1) and (2), which shows a strong temperature dependence and considerable softening for temperatures above about 250K. The predicted transformation between Orowan looping and a shear bypass mechanisms occurs at a temperature of about 220K, which is very consistent with the bypass mechanism shift observed for an edge dislocation with a 3 nm coherent Co

precipitate in the MD simulations, as shown in Fig. 5b. At low temperatures, the structural phase transformation precipitate strengthening from Eq. (2) is greater than that associated with the Orowan strength, and therefore a dislocation bypass mechanism by Orowan looping would be expected as the path of least resistance, consistent with the MD simulation results. The strong linear temperature resistance of the structural phase transformation precipitate strengthening mechanism produces a cross over in the minimum CRSS between the two mechanisms curves at about 220 K. Indeed, for temperatures of 300 and 400 K, the MD simulations reveal that the dislocation interacts and bypasses the precipitate with the expected shear mechanism (Fig. 5b).

Furthermore, we can incorporate an estimate of the phonon drag, or inertial effect, on the dislocation motion by assigning an effective drag stress on the dislocation according to the well-known relation [22],

$$\tau_{\text{drag}} = \frac{Bv}{b} \quad (4)$$

where B is the Friction coefficient, with units of Ns/m^2 , v is the average dislocation velocity and b is the Burgers vector. We have used MD simulations to evaluate the temperature dependence of B , which ranges from about $2 \times 10^{-5} \text{ Ns/m}^2$ at 10 K to $3 \times 10^{-5} \text{ Ns/m}^2$ at 500K as shown in Supplementary Fig. 3, and used an average dislocation velocity of 750 m/s, based on observations from MD simulations, to estimate a drag stress contribution to the overall CRSS. In Fig. 6, this effective resistance to dislocation motion due to phonon drag is plotted by the blue squares, and is motivated by the analysis of Nembach and co-workers [10,11]. The black circles in Fig. 6 represent the

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4 normalized temperature dependent precipitate strengthening obtained from the minimum
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6 resistance of the two strengthening mechanisms from Fig. 5a. A root sum square
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8 superposition of these two contributions to the dislocation resistance results in the curve
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10 plotted with red diamonds as the overall CRSS for a Cu-Co alloy containing 3 nm
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12 diameter, coherent cobalt precipitates and an obstacle spacing of 26.5 nm. The qualitative
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14 features of this predicted CRSS are in remarkably good agreement with the
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16 experimentally determined temperature dependence of the CRSS of Cu-Co alloys
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18 reproduced in Fig. 1. Indeed, we believe that a combination of a dynamic effects on the
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20 dislocation motion due to phonon drag and a temperature dependent precipitate
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22 strengthening can fully explain the observed temperature dependence of the Cu-Co
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24 system, in which a peak CRSS is observed at temperatures between 200 and 250K, and
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26 that the CRSS at 500 K is approximately the same order of magnitude as that at 10K.
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33 The temperature dependence of the normalized CRSS predicted in Fig. 6 is in
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35 excellent agreement with both the MD simulations and the experimental results [10,11].
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37 Thus the MD simulations reveal the existence of a new precipitate strengthening
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39 mechanism in the Cu-Co alloy system, which produces a strongly temperature dependent
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41 precipitate strengthening, in which a reversible structural phase transformation results in
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43 an Orowan looping bypass mechanism of the trailing partial dislocation at low
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45 temperature. When combined with the dynamic dislocation effects described by
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47 Nembach and co-authors [10,11], using a simplified model of a phonon drag contribution
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49 to the CRSS, Fig. 6 shows that the predicted temperature dependence of the CRSS
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51 measured in Cu-Co alloys with small coherent precipitates agrees well with experimental
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53 measurements and MD simulations. Furthermore, the relative absence of temperature
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dependence in alloys with larger incoherent precipitates, can also be understood, since incoherent precipitates with dislocation bypass occurring by an Orowan looping mechanism would have a much weaker temperature dependence than the mixed-mode bypass observed for the smaller, coherent precipitates.

4. Conclusions

Molecular dynamics simulations have been performed to investigate the dislocation interaction and bypass mechanism from coherent, spherical cobalt precipitates in copper. The results of these simulations can be understood based on the underlying dislocation interaction mechanisms with precipitates, and a model has been developed to capture the temperature dependence of the critical resolved shear stress of Cu-Co alloys through the superposition of precipitate strengthening and phonon drag. The major findings are:

- MD simulations reveal a strongly temperature dependent precipitate strength for a coherent, 3 nm diameter Co precipitate in Cu, and the interaction strength also differs for the leading and trailing partial dislocations of both screw and edge dislocations.
- Below 300 K, both the trailing partial dislocations of screw and edge dislocations bypass the coherent, 3 nm diameter cobalt precipitate by Orowan looping. At temperatures above 300 K, the interaction is governed by the expected shear mechanism.
- The Orowan looping results from the structural transformation of the precipitate into the more stable hexagonal close packed structure on the glide plane, and is reversible.
- A model for the CRSS of Cu-Co alloys has been developed based on the superposition of a temperature dependent precipitate strengthening and a contribution

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4 from phonon drag. The model agrees well with both experimental data and these MD
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6 simulations.
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Figure legends

Fig. 1. Temperature dependence of CRSS for Cu-Co alloys. Triangles, diamonds, circles and squares represent 2.23, 1.28, 0.93 and 0 % Co contents, respectively.

Fig. 2. Snapshots of the MD simulation of the edge dislocation glide at 300 K at (a) 16.0, (b) 22.8, (c) 40.0, (d) 44.0, (e) 44.6 and (f) 50.0 ps after applying a shear stress of 100 MPa. Yellow and gray spheres represent Cu and Co atoms, respectively.

Fig. 3. Snapshots of the MD simulations of the edge dislocation glide at 100 K at (a) 15.0, (b) 22.2, (c) 38.8, (d) 41.2 (e) 41.4 and (f) 45.2 ps after applying a shear stress of 100 MPa. Yellow and gray spheres represent Cu and Co atoms, respectively.

Fig. 4. Snapshots of the MD simulations of the screw dislocation glide at 100 K at (a) 25.6, (b) 45.2, (c) 47.8 and (d) 50.0 ps after applying a shear stress of 100 MPa. Yellow and gray spheres represent Cu and Co atoms, respectively.

Fig. 5. (a) Model predictions for the two bypass mechanisms, structural strengthening (black circles) versus the Orowan looping mechanism (blue squares) and (b) mechanism map showing the dislocation bypass mechanism versus temperature and applied stress, as observed by MD simulations of the interaction of a 3 nm, coherent Co precipitate with an edge dislocation. Also shown is the effective CRSS obtained from the MD simulations.

Fig. 6. Predicted temperature dependent normalized CRSS for a Cu-Co alloy containing 3 nm diameter, coherent Co precipitates.

Fig. 1

FIGURES

Fig. 2

Fig. 3

Fig. 4

Fig. 5a

Fig. 5b

Fig. 6