Simulating Microstructure Evolution of Battery Tabs during Ultrasonic Welding

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ABSTRACT

Ultrasonic welding offers ability to weld thin layers of malleable metals at low temperature and low power consumption. During ultrasonic welding, intensive material interactions occur due to the severe plastic deformation (SPD) and frictional heat generation, which leads to the microstructural change. Different grain microstructures have been observed after different ultrasonic welding conditions. Theory of the microstructural evolution was for the first time hypothesized as three regimes, namely SPD, dynamic recrystallization (DRX) and grain growth according to the material thermomechanical loading conditions. A novel metallo-thermo-mechanically coupled model was developed to model the temperature-dependent mechanical deformation and microstructural evolution during the ultrasonic spot welding process. The numerical analysis was carried out with a three-dimensional (3D) finite element model using DEFORM 11.0. The material constitutive model considered cyclic plasticity, thermal softening and acoustic softening. Dynamic recrystallization and grain growth kinetics laws were applied to simulate the microstructural evolution under different welding time durations. The simulation results demonstrated that the essential characteristics of the deformation field and microstructure evolution during ultrasonic welding were well captured by the metallo-thermo-mechanically coupled model. The numerical framework developed in this study has been shown to be a powerful tool to optimize the ultrasonic welding process for its mechanical properties and microstructures.

Keywords: Ultrasonic Welding, Modeling, Microstructure, Dynamic Recrystallization, Grain Growth

1. Introduction

Battery electric vehicles have drawn great attentions in recent years. The battery pack for a battery electric vehicle is assembled from a large amount of battery cells. Due to the virtues of low power consumption, rapid solid-state joining and environment friendliness, ultrasonic spot welding has been applied as a practical and efficient solution for joining of metallic battery tabs to a bus (S. S. Lee et al.,

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2013). Ultrasonic welding is often used to create a joint between thin malleable metals such as aluminum (Al), copper (Cu) and nickel (Ni) (Xu et al., 2016). It is also applied to join multi-layer dissimilar metals with varying sheet thicknesses.

The performance of ultrasonic spot welding has been extensively studied for battery tab joining in recent years. Lee et al. (2013) conducted a thorough experimental analysis of ultrasonic spot welding of copper battery tabs and defined several key weld attributes, i.e., bond density, post-weld thickness, weld nugget size and thermomechanically affected zone size, to determine the weld quality. Their study also revealed that the resultant microstructure and material strength of the weld highly depended on the welding process parameters. Lee et al. (2015) experimentally investigated the performance of multi-layer ultrasonic weld by joining four coupons of Cu with various thicknesses. A high speed imaging technique was used to capture the displacement of horn and different coupons for ultrasonic welding using different knurling tools. The effect of vibration on weld formation from top to bottom layers was investigated from the analysis, which concluded that weld quality deteriorates from top to bottom layers due to less heat generation at the interfaces of bottom layers. Wu et al. (2015) investigated the welding and failure mechanism of the Al/Cu ultrasonic welding using the mechanical testing and microstructural analysis. An online monitoring system was developed using welding power and horn displacement (Lee et al., 2014). The weld quality was evaluated in terms of post-weld thickness and bond density based on the online signals for process control. Zhao et al. (2014) developed a fatigue life cycle model to predict the life of Al/Cu ultrasonic weld tab joints by monitoring electrical resistance. The mechanical response of the Cu or Al/Cu tabs and ultrasonic welding system were studied to understand its effects on the weld quality and to reduce energy loss (Kang et al., 2014a, 2014b).

Considerable research efforts have also been devoted to characterize the thermal field in the weld zone. The thermal contact conductance between thin metal sheets was determined as a function of contact pressure (Chen et al., 2014). The real-time temperature and heat flux change have been measured and monitored near the weld zone using thin-film thermocouples (Zhao et al., 2013) and thin-film micro-sensors (Li et al., 2013). Different weld formations were studied for various welding time durations from 0.6 sec to 1.5 sec. Based on the history of heat flux change rate, Li et al. (2013) proposed a bonding mechanism for ultrasonic welding consisting of three continuous stages within one operation, which were firstly friction heating, then bonding by plastic work, and finally diffusion bonding.

Materials often demonstrate a significant softening phenomenon under ultrasonic loading. The softening effect during ultrasonic spot welding is considered in two main mechanisms of thermal softening and acoustic softening. Thermal softening is attributed to the frictional heat generation from the high frequency vibration. The thermal energy is uniformly absorbed by the metal material. The acoustic softening contributes more on the flow stress reduction. The acoustic energy generated by ultrasonic sonotrode is transmitted to the metal and locally absorbed at defected crystal lattice, e.g. vacancies, dislocations and grain boundaries (Langenecker, 1966). As a result, the activation energy of the dislocation line movement is considerably reduced (Langenecker, 1961). The increased mobility of dislocations drastically attenuates the work-hardening, so flow stress can be extremely reduced.

Numerical modeling studies have been attempted to model the thermomechanical coupling effect during ultrasonic spot welding. Elangovan et al. (2009) developed a two-dimensional (2D) finite element (FE) model for ultrasonic welding of dissimilar materials. In their model, the effective heat generation terms were adopted from a previous study (De Vries, 2004) for modeling heat generation due to deformation and friction under ultrasonic vibration. D. Lee et al. (2013) developed a three-dimensional (3D) thermomechanical FE model and used a combined explicit/implicit multi-step numerical approach to predict ultrasonic spot welding of multi-sheet dissimilar materials (Al and Cu). However, the acoustic softening effect on material flow stress under ultrasonic loading was not

considered in these aforementioned studies.

Siddiq and Ghassemieh (2008) developed a material phenomenological constitutive model to consider the acoustic softening effect in the combined isotropic/kinematic hardening model under cyclic loading. This model was successfully implemented in a 3D thermomechanical FE model for an ultrasonic seam welding process of Al ally 6061 using a sonotrode with smooth cylindrical surface. The temperature-dependent friction coefficient was calibrated and applied to predict the frictional heat generation under ultrasonic vibration. Siddiq et al. (2009) applied this numerical approach to model ultrasonic seam welding of Al ally 3003 and investigated the effects of various process parameters, such as applied load, ultrasonic vibration amplitude, and tool velocity, on weld material response. Siddiq and Sayed (2011) further proposed a micromechanics-based crystal plasticity model by incorporating the phenomenological acoustic softening term and simulated the ultrasonic assisted deformation of both single crystalline and polycrystalline Al materials. With this model development, the workpiece material textural change was simulated for ultrasonic consolidation at sub-micron scale (Siddiq and Sayed, 2012).

Different from ultrasonic seam welding using a smooth cylindrical sonotrode, for ultrasonic spot welding of battery tabs, a sonotrode and an anvil with diamond knurl patterns are used to significantly enhance the welding process capability. During the process, weld forms from compression and ultrasonic in-plane sliding of the diamond knurling tool, which induces severe plastic deformation (SPD) in the workpiece material. Experimental results of ultrasonic spot welding from Lee et al. (2013) showed complex coupling effects among mechanical deformation, heat transfer, and microstructure change for various welding time durations. Their study revealed the material microstructure underwent different evolution routes with varying thermal and deformation histories. There is a great challenge in modeling such a metallo-thermo-mechanical coupled process under ultrasonic vibration. The available numerical approaches in literature are not capable to simulate the complex weld formation and microstructural evolution for the ultrasonic spot welding process.

Our present study is to develop a predictive metallo-thermo-mechanically coupled model to simulate severe plastic deformation and microstructural change during the ultrasonic spot welding process for battery tabs. Multiple 3D coupled thermomechanical FE simulations are conducted with DEFORM 11.0 to simulate the deformed weld shape and temperature change after different process durations. The microstructural evolution and the microhardness change are predicted using a post-processing user routine.

2. Principle of Ultrasonic Welding

The principle of the ultrasonic welding is discussed based on a systematic experimental study carried out by Lee et al. (2013). In their experimental study of ultrasonic welding for tab-bus joining in automotive battery cell, two C11000Cu sheets (99.9% pure) were joined by an AmTech Ultraweld® L-20 high power welder with a maximum output electric power of 4 kW. The top and bottom sheets were 0.4 and 1 mm in thickness, respectively. The bottom sheet was plated by a thin Ni layer (~3 µm thick). The ultrasonic vibration was implemented in the workpiece transverse direction with an amplitude of 30 µm at 20 kHz frequency. The

clamping force was applied along the vertical direction and varied from 40 to 60 psi. Multiple experiments were performed for different welding time from 0.2 to 1.0 sec. Different knurl and anvil patterns were applied in their experiments. All the experimental parameters were listed in Table 1.

Table 1. Experimental conditions (S. S. Lee et al., 2013).

Materials	C11000 Cu (tab) Ni-plated C11000 Cu (bus)
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Coupon thickness (mm)	0.4 mm (tab) 1 mm (bus)
Load (psi)	40, 50, 60
Vibration amplitude (μm)	30

Frequency (kHz)	20
Welding time (sec)	0.2, 0.4 0.6, 0.8, 1.0

The weld joint microstructure was examined near the joint interface. The as-received sheets were rolled and annealed before the welding experiments, which had strain-free grains for both top and bottom coupons as shown in Fig. 1a. Fig. 1b-f examine the microstructures obtained after ultrasonic spot welding under a clamping pressure of 50 psi with varying welding time durations observed by S. S. Lee et al., 2013. It can be recognized that the material microstructure underwent different evolution routes as the welding time increased. For a short welding time of 0.2 sec, a great amount of elongated grains can be seen in Fig. 1b on both side of the joint interface. As the welding time increased to 0.4 sec, the elongated grains became dissolved, and newly formed strain-free-like fine grains can be seen in Fig. 1c. Similar microstructure with newly-formed fine grains near the weld interface was also observed after a 0.3 sec ultrasonic spot welding of Al alloy 6111 under a similar ultrasonic loading condition (Bakavos and Prangnell, 2010). In Fig. 1d, fine equiaxed recrystallized grains were formed with very clear grain boundaries in most area of the specimen cross-section after 0.6 sec welding. As the welding time increased to 0.8-1.0 sec, coarse grains were mainly seen in the specimen as shown in Fig. 1e-f. In addition, a uniform microstructure was formed under these two conditions, while the difference across the weld interface was obvious for the shorter welding durations.

Fig. 1 Microstructure after various welding time durations: a) original microstructure before welding; b) 0.2 sec; c) 0.4 sec; d) 0.6 sec; e) 0.8 sec; f) 1.0 sec. The original images were adopted from (S. S. Lee et al., 2013).

The grain size was measured separately for the top and bottom coupons using the optical micrographs for all the specimens. Fig. 2 shows the measured average grain size from both sides of the

weld line. The grain size of the as-received material was also measured: finer grains of 7.5 μm were observed in the thinner top coupon, while the thicker bottom coupon had a greater grain size of 12.5 μm . Significant grain refinement was observed after 0.2 sec welding. After a welding time of 0.4-0.6 sec, the grain size of about 10 μm was obtained. As the welding time increased to above 0.8 sec, significant grain growth to 30 μm occurred. After welding time of 0.4 sec, a small grain size of 7.6 μm was measured in the top coupon, while a big grain size of 11.6 μm was found in the bottom coupon. However, this difference in grain size between the top and bottom coupons started to diminish during grain growth under a longer welding time duration.

Fig. 2 Grain size measurement

Fig. 3 shows microhardness at different locations on the cross-sectioned of weld joints from these experiments. The micro-indentation hardness tests were performed on the yellow spots. As labeled in Fig. 3, valley is denoted as the more plastically deformed domain under the tip of the knurling tool, while the peak is the less deformed domain. Significant hardness increases can be observed for specimens made from a short welding time duration of 0.2 sec, especially at the valleys. As welding time duration increased from 0.2 sec to 1 sec, the microhardness at the valleys drastically decreased. It became even lower than the original value, when welding time duration increased to 1 sec. Fig. 3 also shows the microhardness of weld joint varied at different locations due to different plastic deformation. For a short welding time duration (less than 0.4 sec), the more deformed valley has a much higher microhardness than that of the peaks. However, as the welding time increased, the difference in microhardness between the more and less deformed domains was significantly reduced or even diminished. The microhardness change was caused by the combined effect of the welding time, severe plastic deformation as well as microstructural evolution during ultrasonic welding.

Fig. 3 Hardness measurement of the joints at different locations with different welding durations.

The changes of microstructure and microhardness as shown in Fig. 1-3 highly depend on the process time duration. A main effect of increasing welding time duration is the increase of process temperature. After the welding time duration, the knurling tools were disengaged from the joints and coupons and a workpiece cooling process took place in air. For a high process temperature with a long welding time duration, it also takes a longer time for the joint to cool down. For a short welding time less than 0.2 sec, the process temperature was most likely low. Work hardening and grain refinement

were significant under SPD at a low temperature condition, while dynamic recovery was relatively slow (Ding and Shin, 2014; Ding et al., 2012). A more severe deformation would lead to a finer grain size and a higher mechanical strength. As the welding time duration increased to 0.4-0.6 sec, more heat was generated and the processing temperature would likely reach the recrystallization temperature range. Sufficient strain energy was stored to enable dynamic recrystallization (DRX) due to deformation. As DRX took place, it provided a softening mechanism after a certain level of strain and resulted in a significant drop of the flow stress to a steady-state level. As the welding time duration increased to 0.8-1.0 sec, the processing temperature would become even higher. As the completion of recrystallization, grain growth took place to reduce the grain boundary area. Given a high processing temperature condition, grain growth would continue even after the welding process. Eventually, the material would be softened and had a uniform coarse-grained structure across the weld interface after grain growth.

Different welding time durations also led to different levels of plastic deformation within the weld zone. During the recrystallization process, the extent of deformation affected the final grain size. A more severe deformation had a higher rate of nucleation than the rate of growth (Sellars and Whiteman, 1979). As a result, the final grain size was reduced by the increased deformation. This explains that a finer grain size existed in the top coupon under more plastic deformation and a coarser grain size existed in the less deformed bottom coupon before grain growth.

Based on the above analysis, the microstructural evolution during ultrasonic spot welding can be classified into three regimes:

- For Regime I under a low processing temperature, SPD is hypothesized as the major mechanism to govern the material response and microstructural evolution.
- For Regime II under a medium processing temperature, DRX is hypothesized as the dominant mechanism for microstructural evolution as well as material flow stress response.
- For Regime III under a high processing temperature, DRX and subsequent grain growth are hypothesized as the dominant mechanisms for microstructural evolution as well as material flow stress response.

The final microstructure is determined by the coupled metallo-thermo-mechanical histories during ultrasonic welding. Therefore, modeling of different mechanisms under different regimes are critically needed to better understand the process of ultrasonic spot welding.

3. Modeling

To study the microstructural evolution during the ultrasonic welding and subsequent cooling process, a 3D metallo-thermo-mechanically coupled model was developed with a commercial FE software package of DEFORM 11.0. A material constitutive model was implemented to calculate the flow stress during high frequency ultrasonic vibration. The microstructural evolution and hardness change due to DRX and the subsequent grain growth were simulated with a post-processing user routine.

3.1 Flow Stress Model under Ultrasonic Vibration

Ultrasonic welding involves high-frequency cyclic loading, thermal effect at the interface and ultrasonic effect due to ultrasonic vibration. Therefore, flow stress should be expressed in combined effect of all three phenomena. The basic constitutive equations for cyclic plasticity model were adopted from uniaxial loading. The total strain is the sum of elastic and plastic strain tensor:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{el} + \boldsymbol{\varepsilon}^{pl} \quad (1)$$

Flow stresses at any step of the simulation are calculated using the elastic stress strain relation:

$$\underline{\sigma} = \mathbf{D}_{el} \underline{\varepsilon}^{el} = \mathbf{D}_{el} (\underline{\varepsilon} - \underline{\varepsilon}^{pl}) \quad (2)$$

where $\mathbf{D}_{el}$ is the elasticity tensor. The yield surface is defined by modified Chaboche model, which is considered more accurate for cyclic loading condition (Krishna, 2009).

$$F = |\underline{\sigma} - \underline{\alpha}| = \sigma_0 + R \quad (3)$$

where σ_0 is initial yield stress, $\underline{\alpha}$ is the term related to back stress tensor due to kinematic hardening, and R is the term related to isotropic hardening. The plastic strain during deformation process is given by

$$d\underline{\varepsilon}^{pl} = d\lambda \frac{\partial F}{\partial \underline{\sigma}} \quad (4)$$

where $d\lambda$ is plastic multiplier which satisfies the following Kuhn-Tucker type consistency conditions.

$$F \leq 0; d\lambda \geq 0; d\lambda \cdot F \cong 0 \quad (5)$$

The expansion of yield surface due to isotropic hardening can be expressed as an exponential function of accumulated plastic strain (Siddiq and Sayed, 2012):

$$R = Q(1 - e^{-b\bar{\varepsilon}^{pl}}) \quad (6)$$

where Q and b are material constants. Q is the maximum change of yield surface due to isotropic hardening and b is the rate at which yield surface changes with accumulated equivalent plastic strain $\bar{\varepsilon}^{pl}$. For nonlinear kinematic hardening, the rate of back stress ($\underline{\alpha}$) is given by

$$\dot{\underline{\alpha}} = C \frac{1}{\sigma_0} (\underline{\sigma} - \underline{\alpha}) \dot{\varepsilon}^{pl} - \gamma \underline{\alpha} \dot{\varepsilon}^{pl} \quad (7)$$

where C and γ are material constants from cyclic testing. C stands for the kinematic shift of yield surface and γ stands for the rate at which saturation value of kinematic hardening decreases with increasing plastic strain. $\sigma_0 = \sigma_y + R$, where σ_y is the yield stress for zero plastic strain. The back stress can be integrated from Eq. 7 for uniaxial case:

$$\alpha = \frac{C}{\gamma} (1 - e^{-\gamma \bar{\varepsilon}^{pl}}) + \alpha_1 e^{-\gamma \bar{\varepsilon}^{pl}} \quad (8)$$

where α_1 is obtained from stabilized cycle and is given by $\alpha_1 = \sigma_1 - \sigma_s$ with σ_1 is the stress at the start of the stabilized cycle and σ_s is the yield stress at stabilized cycle.

$$\sigma_s = \frac{\sigma_1 + \sigma_n}{2} \quad (9)$$

where σ_1 and σ_n are the stress at the start and end of stabilized cycle.

A phenomenological softening term $[(1 - dE_u)^e]$ dependent upon the ultrasonic energy density per unit time has been introduced in the relations of isotropic and kinematic hardening terms to demonstrate the ultrasonic softening effect on yield stress (Siddiq and Ghassemieh, 2008). The thermal softening is included in the flow stress model by embedding the temperature term of $\left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right]$ (Johnson and Cook, 1983). By including both thermal softening and acoustic softening, the modified equations of isotropic and kinematic hardening are given by (Siddiq and Sayed, 2012):

$$R_{ultrasonic} = [Q(1 - e^{-b\bar{\varepsilon}^{pl}})] \left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right] [(1 - dE_u)^e] \quad (10)$$

$$\underline{\alpha}_{ultrasonic} = \left[\frac{C}{\gamma} (1 - e^{-\gamma \bar{\varepsilon}^{pl}}) + \alpha_1 e^{-\gamma \bar{\varepsilon}^{pl}}\right] \left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^m\right] [(1 - dE_u)^e] \quad (11)$$

where d and e are the material constants related to ultrasonic softening and E_u is the ultrasonic energy density per unit time transferred from ultrasonic vibrator to the material. The constant values of copper are given in Table 2. These values were calibrated from experimental work for cyclic loading on copper (Bower, 1989), except the value of e was adopted from the previous simulation work for ultrasonic seam welding (Siddiq and Ghassemieh, 2008). E_u was adopted as $3.5 \times 10^5 \text{ W/m}^2$ for the top coupon, while a smaller E_u of $8.1 \times 10^4 \text{ W/m}^2$ was accessed for the bottom coupon subjected to less acoustic softening. The bottom coupon was relatively far away from the knurling tool, which was mounted on the ultrasonic horn. Based on the literature search and observations in (Lee et al., 2015), the amplitude of ultrasonic vibrations decreased for the bottom coupon.

Table 2. Material parameters in the flow stress model (Bower, 1989; Siddiq and Ghassemieh, 2008).

Q (MPa)	b	C (MPa)	γ	m	T_m (°C)	T_r (°C)	d (m ² /W)	E_u (W/m ²)	e
40	11	22300	340	1.09	1083	25	1.3e-6	3.5e5 for Top 8.1e4 for Bottom	2

3.2 Modeling for Microstructural Evolution

To predict the microstructural evolution correctly, modeling approach must comprehend the process physics under different regimes during ultrasonic spot welding. For grain refinement by SPD under Regime I, a dislocation density-based computational approach has been established by the authors to model the microstructural evolution and strength enhancement during various SPD processes, such as multi-pass cold rolling (Ding et al., 2012) and large strain orthogonal cutting (Ding and Shin, 2014; Ding et al., 2011). The nucleation of dislocations due to deformation, annihilation of dislocations due to dynamic recovery, and interaction of dislocations between the dislocation cell interiors and cell walls can be evaluated based on the deformation process state variables (Shen et al., 2015a, 2015b). The dislocation density-based material plasticity model was compatible with the material constitutive models developed under various conditions of strain, strain rate, and temperature. With the developed dislocation density-based numerical solution, the modeling effort for Regime I is omitted in this work. Modeling of microstructural evolution under Regimes II and III are described as follows.

As the rise of Regime II, the refined grain structure from SPD is rapidly replaced by DRX. The strain hardened weld is softened by DRX and subsequent grain growth during Regimes II and III. The dynamic recrystallization and grain growth were coupled together in this analysis. The model for either regime would be enabled if specific conditions were fulfilled. As the increase of welding time duration, the DRX-dominated Regime II would arise first. The microstructural evolution of copper by DRX has been studied by researchers for a wide range of temperatures (Brown and Bammann, 2012; García et al., 2007). A critical temperature is required for the onset of DRX. In this study, the starting temperature of DRX was assumed as $0.4T_m$, which is about 270 °C for Cu. When this starting temperature is reached, the onset of DRX occurs at a critical equivalent plastic strain. As soon as DRX occurs, the softening effect induced by DRX becomes noticeable, and the flow stress increase rate becomes slower until the peak stress value is reached (Behnagh et al., 2015). After reaching the peak value, the flow stress curve drops rapidly to a steady-state region as strain further increases.

A kinetic model was developed to capture the microstructural evolution during a warm/hot deformation process. The progress of DRX is characterized as the change of the volume fraction of DRX (Yanagimoto et al., 1998). The DRX kinetic model is defined by (DEFORM, 2014):

$$\varepsilon_c = a_2 \varepsilon_p \quad (12)$$

$$\varepsilon_p = a_1 d_0^{n_1} \varepsilon^{m_1} \exp\left(\frac{Q_1}{RT}\right) \quad (13)$$

$$\varepsilon_{0.5} = a_5 d_0 \varepsilon^{m_5} \exp\left(\frac{Q_5}{RT}\right) \quad (14)$$

$$X_{DRX} = 1 - \exp\left[-\beta_d \left(\frac{\varepsilon}{\varepsilon_{0.5}}\right)^{k_d}\right] \quad (15)$$

where ε_c is the critical strain for the onset of DRX, ε_p is the peak stress strain corresponding to the maximum flow stress, $\varepsilon_{0.5}$ denotes the strain at 50% recrystallization, d_0 is the initial grain size, T is the process temperature in K, and X_{DRX} is the volume fraction of DRX. R is the ideal gas constant of 8.314 J/mol·K. β_d , k_d and a_i , n_i and m_i ($i = 1, 2, \dots, 9$) are material constants in each equation, and Q_i is a modified activation energy. During the recrystallization, the averaged grain size (d) after DRX can be predicted by a mixture rule:

$$d = d_o - (d_o - d_{DRX})X_{DRX} \quad (16)$$

$$d_{DRX} = a_8 d_o \varepsilon^{m_8} \exp\left(\frac{Q_8}{RT}\right) \quad (17)$$

where d_{DRX} is the predicted grain size after DRX. The initial grain size d_o was assumed uniformly distributed in the coupons.

As recrystallization completes, grain growth would take place to reduce the grain boundary area per unit volume if the temperature is higher than the grain growth starting temperature (Sellars and Whiteman, 1979). In this study, the grain growth starting temperature was assumed as $0.5T_m$, which is 406 °C for Cu. Grain growth was considered to end as temperature dropped below 406 °C during the cooling step. The final grain size due to grain growth, d_g , is given by:

$$d_g = \left[d_0^{m_9} + a_9 t \cdot \exp\left(\frac{Q_9}{RT}\right)\right]^{1/m} \quad (18)$$

where t is the time duration for temperature above grain growth starting temperature, which also includes the time duration during the cooling stage. The relationship between hardness and average grain size after welding is represented by Hall-Petch equation (Callister and Rethwisch, 2012):

$$H = H_o + k d^{-\frac{1}{2}} \quad (19)$$

where H is the microhardness of the material, H_o and k are material constants determined from the relationship of measured grain size and hardness. All the aforementioned material constants were calibrated based on the previously reported experimental results (Brown and Bammann, 2012; S. S. Lee et al., 2013). These values are listed in Table 3. Other necessary mechanical and physical properties of copper are given in Table 4.

Table 3. Model parameters to predict grain growth and microhardness.

β_d	k_d	a_1	n_1	m_1	a_2	Q_1 (kJ/mol)	Q_5 (kJ/mol)	Q_8 (kJ/mol)
0.72	4.1	0.0003	1	0.1029	0.81	20.27	15.39	-44.33
a_5	m_5	a_8	m_8	a_9	m_9	H_o (HV)	Q_9 (kJ/mol)	k (HV $\sqrt{m}$)
0.0011	0.0781	711.45	0.15	25.29	-0.225	56.1	4.027	0.0487

Table 4. Mechanical and Physical Properties for Pure Cu (Erickson, 1990).

Property	Value
Density (kg/m^3)	8890
Young's modulus (GPa)	115
Poisson's ratio	0.33
Melting point ($^{\circ}\text{C}$)	1083
Thermal conductivity ($\text{W/m}\cdot^{\circ}\text{C}$)	391
Heat Capacity ($\text{J/Kg}\cdot^{\circ}\text{C}$)	385
Thermal expansion ($\mu\text{m/m}\cdot^{\circ}\text{C}$)	17

3.3 Process Modeling

Fig. 4a shows the 3D modeling configuration in DEFORM 11.0 for the ultrasonic spot welding experiment. The typical knurl and anvil pattern designs are shown in Fig. 4b-c, respectively. For the modeled condition, both knurl and anvil had the diamond pattern with 4×4 knurling tips to treat an area of $5\times 5\text{ mm}^2$. Both knurl and anvil were treated as rigid bodies in this model. The top and bottom sheets were 0.4 mm and 1 mm in thickness, respectively. The thin Ni layer of $3\text{ }\mu\text{m}$ was not considered in this model. Clamping force was applied at the back of the knurling tools along the vertical direction. The knurl can move along the vertical direction, while the anvil was fixed in all the degree of freedoms. Multiple simulations were conducted with varying welding time durations from 0.2 sec to 1.0 sec. After the welding step simulation, the tools were disengaged from the joints and coupons and a cooling step was simulated for the workpiece using a natural convection ($20\text{ W/m}^2\cdot\text{K}$) condition. The modified Chaboche yield criterion was applied effectively by defining kinematic and isotropic hardening rule separately. The hardening rule was specified as kinematic with the back stress defined within the whole coupon domain. The sum of isotropic hardening term R and initial yield stress σ_o was given as tabular data in DEFORM, which were calculated from various strains and temperatures.

Fig. 4 FE modeling setup for ultrasonic welding: a) FE configuration; b) knurl pattern; c) anvil pattern.

Ultrasonic vibration was not directly modeled for the horn in this work to save computational cost. When ultrasonic vibration was implemented for the knurling tool, computational cost was too high to complete even a very short period of welding process. In this study, the effect of ultrasonic vibration was considered as acoustic softening on flow stress and frictional heat generation. The acoustic softening effect by ultrasonic vibration was modeled as in Section 3.1. The effect on frictional heat generation was considered for both friction coefficient and heat generation.

During ultrasonic welding, heat generation mainly occurs at the interface between the two sheets from both mechanical deformation and friction (Elangovan et al., 2009). Thus, a constant surface heat flux was applied in this model at the interface between the top and bottom copper sheets. The applied surface heat flux was 18.15 W/mm^2 in this model, which was calibrated by comparing the simulated temperature histories at different locations to the measurement (Li et al., 2013). The friction coefficients between the knurling tools and workpieces were considered to be temperature-dependent. The friction coefficient was reported to increase with temperature up to a certain temperature then start to decrease (Zhang et al., 2006). The temperature dependency of friction coefficient was given by:

$$\mu = \mu_0 (8.485 \times 10^{-10} T^4 - 8.842 \times 10^{-7} T^3 + 1.969 \times 10^{-4} T^2 - 9.762 \times 10^{-3} T + 1.12) \quad (20)$$

where μ_0 equals to 0.39, which is the kinetic friction coefficient at room temperature between copper and steel (Rabinowicz, 1951)

To predict the continuous grain growth after ultrasonic welding, a cooling step was simulated with a natural convection ($20 \text{ W/m}^2\text{-K}$) applied after the welding step. For the experiments with longer welding time durations of 0.8 and 1.0 sec, the simulated thermal history for both welding and cooling steps was used to predict the final grain size due to grain growth. A post-processing user routine programmed in FORTRAN was implemented to predict the microstructural evolution and microhardness change as given in Section 3.2. Fig. 5 shows the flow chart of the post-processing user routine. As aforementioned, the starting temperature of DRX and grain growth were adopted as $0.4T_m$ and $0.5T_m$, respectively, i.e., 270 and 406 °C for Cu. If the temperature was higher than 406 °C, the grain growth would continue through the cooling step after the welding step until the temperature dropped below 406 °C.

Fig. 5 Flowchart for post-processing user routine.

4. Simulation Results and Discussions

Fig. 6 shows the simulated 3D Von Mises stress distributions on both top and bottom coupons at the welding time of 1.0 sec. A 4×4 array of indents can be seen in the weld zone on the top sheet. The stress in the top sheet was lower than that of the bottom sheet. This was resulted from different magnitudes of acoustic softening. More acoustic softening was applied in the top sheet because significantly more ultrasonic energy was absorbed in the top sheet.

Fig. 6 Effective stress distribution at 1.0 sec ultrasonic welding in: a) top coupon; b) bottom coupon.

Simulated temperature distributions are shown in Fig. 7 for both welding step (1.0 sec welding time duration) and cooling step. The weld joint area was predicted to have a relative uniform temperature distribution of about 500 °C at the end of 1.0 sec welding duration. This average temperature was determined for welding processes with various welding time durations. Fig. 7b shows the temperature prediction during the cooling step with the knurling tools disengaged from the coupons. Fig. 8 compares the simulated temperatures with the experimental measurements undertaken by a welding time duration of 0.4 sec (Li et al., 2013). Thermocouples could not be directly applied within the weld zone but were attached to the top Cu coupon at about 1.5 mm away from the weld zone, denoted as P1 and P2 as can be seen in Fig. 8. The temperature histories at these thermocouple locations were tracked from the simulation result. Under the friction heat flux of 18.15 W/mm², the simulated temperature histories agreed well with the experimental measurements for both thermocouple locations. This validated the accuracy of temperature prediction in this analysis.

Fig. 7 Temperature distribution of 1 sec ultrasonic welding simulation: a) at 1.0 sec; b) during cooling

Fig. 8 Simulated temperature histories at two locations on the Cu coupon during a 0.4 sec welding experiment. The temperature measurements were adopted from (Li et al., 2013).

Fig. 9 shows the simulated microstructural variables in terms of volume fraction of DRX, grain size, and microhardness after 1 sec welding and subsequent cooling, which were calculated using the post-processing user routine. As shown in Fig. 9a, DRX completed in most area of the top coupon within the weld zone due to the more plastic deformation, while DRX only occurred near the anvil indents in the bottom coupon due to less deformation. Grain size was determined from the temperature history, which was predicted about $34.7 \mu\text{m}$ in the weld zone and smaller in the surrounding area. Accordingly, the microhardness followed the reversed trend of the grain size. A low hardness was predicted in the welding zone because of the coarse grains and became higher in the surrounding area.

Fig. 9 Microstructure prediction for 1.0 sec welding

The simulation results of process temperature under different welding conditions were shown in Fig. 10. Fig. 10a shows the predicted process temperature, i.e., average temperature along the joint interface, for welding time durations of 0.6 and 1.0 sec. The process temperature increased very fast during the welding step, and then dropped quickly within the first 10 sec of the cooling step. In Fig. 10, microstructural evolution regimes were color highlighted by different temperature ranges. For instance, for 1.0 sec welding time duration, the material microstructure underwent different stages of evolution following the loading history, i.e., firstly Regime I SPD, then Regime II DRX, and finally Regime III grain growth. Because of the intensive heat generation under 1.0 sec welding duration, the process temperature was predicted to be above 406 °C for 16 sec, during which grain growth occurred. While the temperature increase was only increased to about 400 °C under the welding time duration of 0.6 sec, grain growth did not occur under that condition.

Fig. 10b summarizes the predicted process temperatures and microstructural evolution regimes under different welding time durations. For the short welding time duration of 0.2 sec, the process temperature did not reach the DRX starting temperature (40% of the melting point T_m , or about 270 °C for Cu), microstructural evolution was governed by SPD. For welding time of 0.4-0.6 sec, the process temperatures were in the range of the DRX (0.4-0.5 T_m , or 270-406 °C for Cu), which dominated the microstructural evolution. For welding time of 0.8 and 1.0 sec, the process temperature exceeded the starting temperature of grain growth (0.5 T_m , or 406 °C for Cu), and the final grain size was determined by the grain growth mechanism. These findings agreed well with the experimental observations on microstructural evolution in Section 2 and validated the hypotheses in microstructural evolution.

Fig. 10 Comparison of the simulated temperature histories and peak temperatures: a) Temperature history in both welding and cooling step (welding time of 0.6 and 1.0 sec); b) welding time effect on the simulated process temperatures.

Fig. 11 shows the predicted weld joint geometry under various welding time durations. The model predictions show more compacted joint with welding time increasing. Larger knurling indents were predicted in the top sheets than the bottom sheet. These modeling results matched well with the experimental results. Fig. 12 further examines the weld thickness from the simulations, which was defined as the thinnest distance from the top to bottom surface of the weld as shown in Fig. 11. The model accurately predicted the weld thickness under different welding time duration, which reduced from 1.4 mm achieved at 0.2 sec welding duration to about 0.6 mm after 1.0 sec welding.

Fig. 11 Simulated deformed geometry under different welding durations compared with the experimental results in (S. S. Lee et al., 2013).

Fig. 12 Simulated weld thickness under different welding durations compared with experimental measured weld thickness in (S. S. Lee et al., 2013).

As a final note, the bonding between two coupons is not captured in this model. As a result, the simulated stress and strain field is not continuous across the weld interface, especially when the uniform microstructure is formed after a longer welding time. The current model is unable to capture this bonding physics. The future goal of this study is to integrate this model into a multi-scale model to capture the local change of weld interface, e.g. inter-lock formation between the layers, and material diffusion across the weld interface. In that case, the grain structure evolution due to DRX and the subsequent grain growth would be more accurate. Again, the application of ultrasonic softening effect needs to be improved in the future model as well. A flow stress user subroutine is required to apply the acoustic softening in the weld zone, not the bulk material of the coupon.

5. Conclusions

The microstructural evolution mechanisms for ultrasonic spot welding were first hypothesized as three regimes of SPD, DRX and grain growth according to the material thermomechanical loading conditions. A novel metallo-thermo-mechanically coupled 3D FE model was successfully developed for ultrasonic spot welding to model both weld formation and microstructural evolution. A combined isotropic/kinematic hardening flow stress model with an

acoustic softening term was implemented to predict the material response under the high frequency ultrasonic vibration. Using a post-processing user routine, a kinetics model was implemented to predict the material microstructural evolution under DRX and grain growth.

The simulated weld zone geometry agreed well with the experiments. The simulations demonstrated that the process temperature during ultrasonic welding was highly dependent on the welding time duration. For welding time duration longer than 0.8 sec, weld material underwent three different stages of SPD, dynamic recrystallization, and grain growth. The final distributions of grain size and consequential microhardness were predicted based on the thermomechanical solution fields and agreed well with the experimental measurements. The simulation results validated the hypotheses proposed in microstructural evolution during ultrasonic welding. In the future work, this numerical framework will be applied for ultrasonic spot welding of dissimilar materials, e.g. Al/Cu tabs, to simulate the weld formation and complicated microstructural evolution.

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