VIII International Conference on Computational Methods for Coupled Problems in Science and Engineering
COUPLED PROBLEMS 2019
E. Oñate, M. Papadrakakis and B. Schrefler (Eds)

A MOLECULAR DYNAMICS STUDY OF THE INTERFACE TEMPERATURE IN ULTRASONIC METAL WELDING

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Key words: Molecular Dynamics Simulations, Ultrasonic Metal Welding, Temperature Evolution, Coupled Problems

Abstract. In this study, mechanical and thermal behavior of the mating interface during ultrasonic metal welding is investigated using molecular dynamics (MD) simulations. In ultrasonic welding process, the reciprocating motion of the sonotrode together with the application of the external pressure on the mating parts are the sources of friction heat generation, high temperature gradient at the interface and plastic deformations.

The rapid process of ultrasonic welding, which takes a few seconds at the longest, involves coupled mechanical and thermal processes. Therefore, MD simulations have been employed to elucidate the nano-mechanics of this complex coupled process within the picosecond timescale. To this end, the atomic scale simulations of the microstructure at and in the vicinity of the mating interface have been carried out.

This contribution addresses the interactive effects of the process parameters on the interface temperature evolution and the diffusion behavior of the interface atoms at the atomic scale. The results of this work are compared to the results from macro scale investigations.

1 INTRODUCTION

Ultrasonic metal welding (USMW) is a solid state consolidation process, during which the growing interface temperature is far below the melting point of the participating metals. During this process, the formation of a bond occurs through a combined effect of the applying pressure normal to the mating parts and the high frequency frictional vibrations of a sonotrode on top of the mating parts. Formation of the bond during the USMW involves moderate to strong plastic deformations as well as friction heat generation and softening of the material at the vicinity of the bond interface. Different aspects of the USMW process have been studied over decades. Microscopic inspections of the bond as

well as real time monitoring of the bond formation and the interface temperature gradient have been carried out to better understand the role of the process parameters in this complex process. Krzanowski [1] observed dynamic recovery or recrystallization in aluminum wires during ultrasonic bonding. Hazlett and Ambekar [2] stated that four bonding mechanisms may occur during ultrasonic welding depending on the mating parts, such as melting of the interface, mechanical interlocking, interfacial atomic forces and interfacial diffusion. Elangovan et al. [3] stated that an increasing clamping force decreases the generated interface temperature and leads to formation of the work piece rather than welding. Ding and Kim [4] showed that a higher bond force results in an insignificant higher temperature rise and does not necessarily result in a better wire bondability. Mostafavi et al. [5] investigated the microstructure of different weld samples under the influence of different pressures and vibration amplitudes of the welding sonotrode. They realized that for a high welding pressure, the boundaries at the contact regions of the aluminum strands are recognizable even after the process ends. They also stated that increasing the vibration amplitude in USMW of multi-strand single core aluminum cables is more efficient in interface temperature rise than increasing the applied pressure. Bai and Yang [6] gave an approximately linear relation between the deformation of surface asperities and ultrasonic vibration amplitude.

However, in-situ investigations of the interface temperature and observation of the bond formation require a big amount of time and precise measuring techniques. Therefore, in recent years MD simulations have been employed to simulate the nano-mechanics of many mechanical processes. Patil et al. [7] proposed a non-linear wear law in disc-pad braking system. Chen et al. [8] studied the microstructure evolution, heat dissipation and generation of mixing layers in the region near the contact interface during nanoscale friction. Chen et al. [9] studied the atomic structure and computed the interfacial energy in Ni-Cr alloys by means of MD simulations. Jiao et al. [10] established an atomic model for the study of linear friction welding between Ni and Al, where they studied the flattening of the surface roughness and the pore closure during the process. Song et al. [11] studied plastic deformation and atomic diffusion behavior in the process of linear friction welding between dissimilar Ti-based alloys.

Various theoretical and numerical models have been proposed in order to study the mechanism of the bond formation and the change in interface temperature, most of which are based on fundamentals of continuum mechanics.

This study employs MD simulations to investigate the nano-mechanics of the interface. The coupled effect of two parameters, namely constant sliding velocity and compression rate on the interface temperature and diffusion behavior of the interface atoms are discussed.

2 SIMULATION METHOD

MD simulations are carried out to discuss the effect of compression rate and sliding velocity on the nanostructure of the interface. In the MD simulations method, atomic

trajectories are obtained through integrating the classical Newtonian equations of motion for a system of N atoms as particles. A force field or potential is used to compute the forces between the atoms in those equations. The velocity and the positions of the atoms are updated based on their interaction potentials.

2.1 Computational model and boundary conditions

MD simulations are performed inside LAMMPS (Sandia National Laboratories)[12]. The velocity-verlet algorithm is used for the numerical integration of the Newtonian equations of motion. For the purpose of visualization of the atomistic simulation data, the open visualization tool Ovito [13] is used. The simulation box consists of two blocks of a monoatomic aluminum FCC structure. The box is filled with a total number of 322,873 atoms. Fig. 1 (left) shows the geometry of the structure. Each block has the dimensions of 60.75×40.5×16.2 Å^3. Three types of atom description are set for the computational model, namely rigid atoms, thermostat atoms and Newtonian atoms. The region of rigid moving atoms moves as a single entity. The thermostat atoms were used to ensure heat dissipation during sliding.

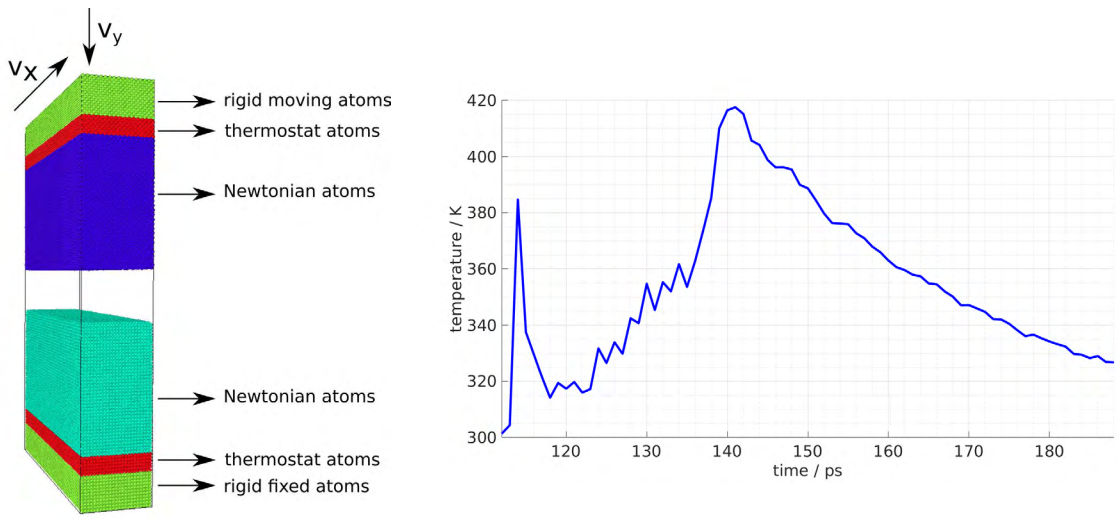

Figure 1: Geometry of the model (left), temperature evolution of the interface (right)

Pressure of the sonotrode and the amplitude of the vibrations are translated into compression rate and sliding velocity in this study. In a reference model the rigid atoms of the upper block are moved at a constant compression rate $v_y = 0.7$ Å/ps and a constant sliding velocity $v_x = 0.9$ Å/ps. The computation is set for 88000 steps with a time step of 0.001 ps. Finally, cool down of the model is set for another 50000 steps.

2.2 Applied methodology

In the present work, the embedded atom method (EAM) interatomic potential developed by Mishin et al. [14] is used (see Eqn. 1). This interatomic potential gives a better description of metallic atoms interactions than a two-body potential and accounts for the effect of electron density surrounding each atom and accurately modeling the surface energy [8].

$$U_{EAM} = \sum_{i}^{N} \left[F_i(\rho_i) + \frac{1}{2} \sum_{j \neq i}^{N} \phi_{ij}(r_{ij}) \right] \,,\ \rho_i = \sum_{j \neq i}^{N} \rho_j(r_{ij}) \,, \tag{1}$$

where i, j describe the types of the atoms, r_{ij} is the scalar distance between atoms i and j and ϕ_{ij} is the pairwise interaction potential. ρ_i is the electron density of atom i due to all its neighbors and $F_i(\rho_i)$ illustrates the energy arising from embedding atom i in an electron gas of density ρ_i.

In a MD computational model, kinetic energy and potential energy of each atom can be calculated at any particular time step. In order to compute the temperature as a global quantity, temperature must be averaged over a certain number of atoms. To this end, kinetic energy of a system with N atoms as in Eqn. 2 is set equal to the kinetic energy from Eqn. 3, which results in the thermodynamic temperature of the system as in Eqn. 4.

$$U_{KE} = \frac{1}{2} \sum_{i}^{N} m_i v_i^2 \,, \tag{2}$$

$$U_{KE} = \frac{3}{2} N k_B T \,, \tag{3}$$

$$T = \frac{1}{3} \frac{m}{N k_B} \sum_{i}^{N} v_i^2 \,, \tag{4}$$

where k_B is the Boltzmann constant.

3 RESULTS AND DISCUSSION

The effect of a percentage-wise increase in compression rate and sliding velocity is studied. In each simulation only one of these two parameters is varied.

3.1 Temperature evolution of the interface atoms

Figure 2 shows the snapshots of the interface temperature once the upper block reaches the lower block. An initial sudden increase of the interface temperature occurs due to the high atomic repulsion energy. This can be seen on the graph in Fig. 1 as well. A global maximum of the interface temperature is achieved at the end of the process. After

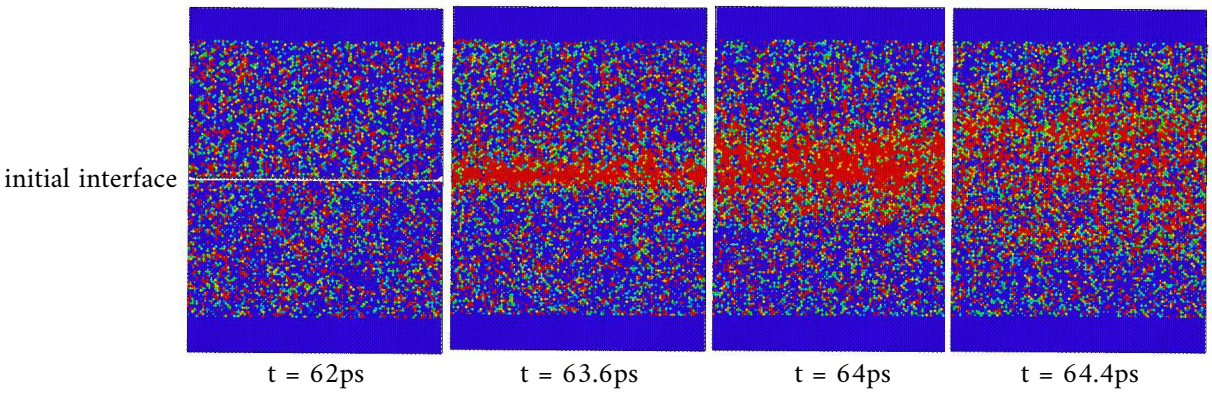

Figure 2: Snapshots of the interface temperature evolution

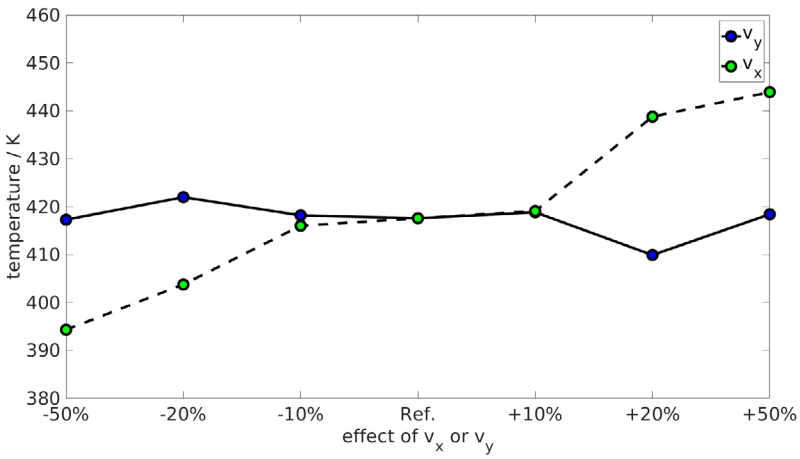

Figure 3: Interface temperature dependency on v_x and v_y

removing v_x and v_y, cool down of the interface takes place and the interface temperature monotonically decreases (see Fig. 1).

As shown in Fig. 3, increasing v_x increases the interface temperature, whereas a clear pattern for the interface temperature change with increasing v_y cannot be recognized.

3.2 Diffusion behavior analysis

Fig. 4 shows the mean square displacement (MSD) of the middle atoms at the interface. To this end, the total squared displacement from the original position of each atom, $(dx^2 + dy^2 + dz^2)$, summed and averaged over all the interface atoms is given in Eqn. 5. The slope of the MSD vs. time is proportional to the diffusion coefficient of the atoms at the interface. As Hazlett and Ambekar [2] claimed, there may be grain boundary diffusion across the bond interface rather than bulk diffusion during the bond formation process. Increasing the sliding velocity helps the atom transfer and diffusion. On the

contrary, increasing the compression rate prevents the atom transfer and does not change the diffusion process significantly.

$$r^2(t) \quad = \frac{1}{N}\left[\sum_i^N |r_i(t) - r_i(0)|^2\right] . \tag{5}$$

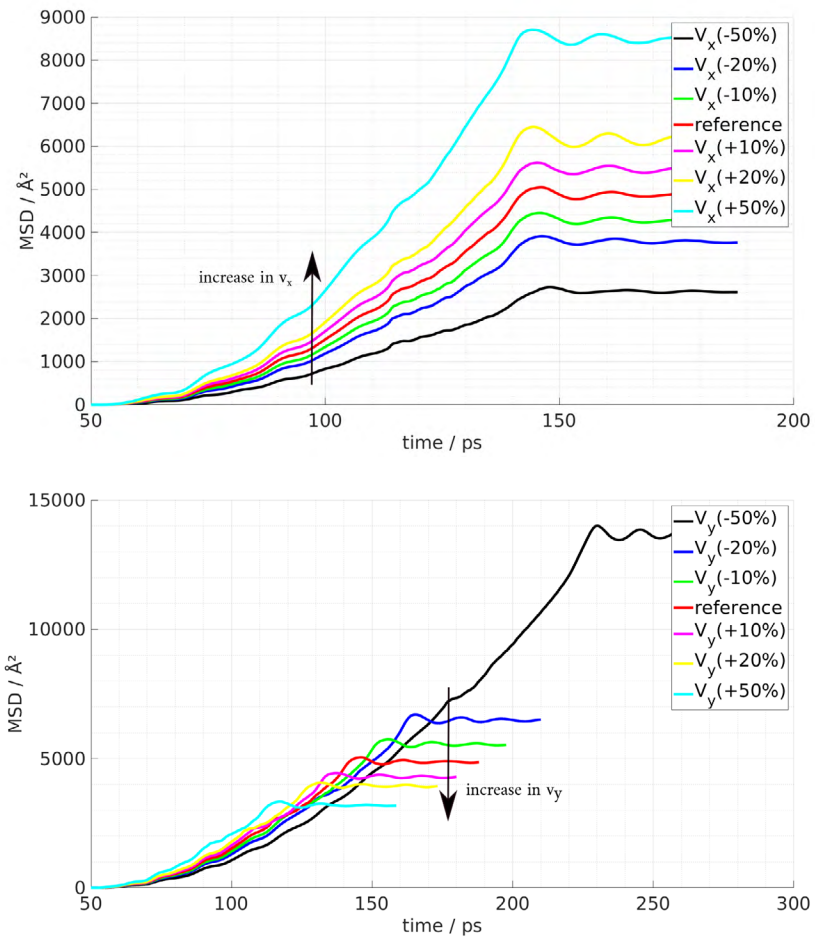

Figure 4: Change in MSD of the interface atoms with v_x (top) and v_y (bottom)

3.3 Correlation between MD, experiments and FE simulations results

In our previous work, results from experiments and FE simulations regarding the interface temperature have been reported in detail [5]. Fig. 5 shows the mean values of the interface temperature for different couples of process parameters in USMW of multi-strand single core aluminum cables from experiments and FE simulations. As shown, increasing the vibration amplitude increases the interface temperature continuously, due to the effective friction heat generation. Increasing the applied pressure increases the interface temperature due to plastic deformations, until a threshold value is reached. A high temperature at the bonding interface is not the only crucial factor in formation of a good bond in USMW, but also the frictional sliding motion of the parts against each other is important as it disperses impurities, oil and metallic oxides at the interface effectively and leaves clean parts for bonding. The results from the simplified atomic scale simulations in the current study are in good agreement with these results from experiments and FE simulations.

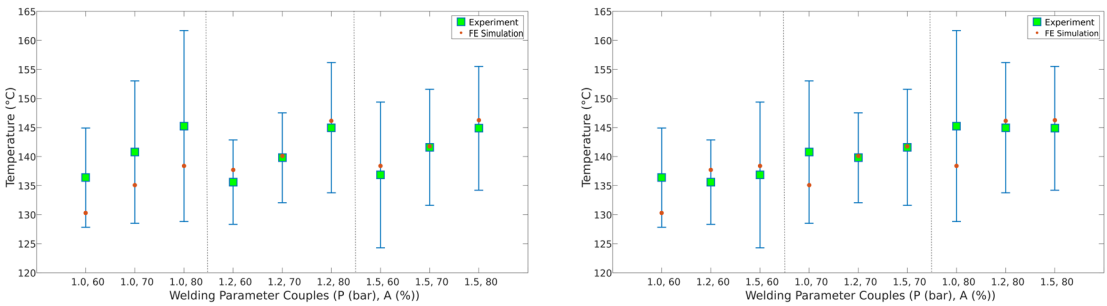

Figure 5: Interface temperature for different couples of process parameters [5]

4 CONCLUSIONS

A study of the mating interface in USMW is done through MD simulations. The main conclusions and achievements of this study are summarized as follows:

- Interface temperature increases as sliding velocity increases. With an increase in the compression rate, interface temperature stays nearly constant.
- Atomic diffusion at the interface increases as sliding velocity increases.
- MD simulations confirm the effect of process parameters on the interface temperature, which has been established by experiments and FE simulations.
- MD simulations are capable of describing the mechanical and thermal characteristics of the interface at nanoscale.

Material and process related parameters obtained from atomistic simulations can be integrated in multi-scale approaches as in [15], where a link between molecular and continuum models of brittle fracture was proposed.

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