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Atomistic Simulation of the Explosion Welding Process**

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We study explosion welding process on the atomic level using molecular dynamics simulations. Our simulations show that jet formation—considered necessary for good bonding—is correlated with the instantaneous melting of the interface region. Moreover, we observe peeling off of material (up to 4 nm) from the bonded surfaces. Finally, the structure of the material immediately after the bonding process is observed to be nanocrystalline with crystal sizes of 10–20 nm.

Explosive welding (EXW) is an industrial process used to join metals together.[1,2] It is a well established method and has been in use for several decades. In the process, welding occurs in a high velocity collision between metal plates, achieved by using chemical explosives. Figure 1(a) shows the schematic arrangement of the plates in EXW. The clad layer is covered with explosive which is ignited from a point or an edge. The detonation front imposes a momentum to the clad layer which—after plastic deformation—collides with the fixed base metal. The most important process parameters are the cladding plate collision velocity v_P, and the collision angle β. These are controlled by adjusting the amount and quality of the explosive and the stand-off distance y_0. In the EXW processes used in the industry the collision velocity is typically of the order of kilometer per second. Clad layer thicknesses t can be up to centimeters and the total area of welded surface can be several square meters.

The advantages of EXW include that it is a ''cold welding'' process and thus free of some of the mechanical and thermodynamic limitations of traditional welding, that it can be used to join almost any pair of metals, including those not weldable by conventional methods, and that it produces a very strong bond, that is often stronger than the weaker of the materials. The joined parts need not be specifically melted for the bonding to take place. This minimizes the formation of intermetallic—often brittle—phases near the interface. EXW is particularly suitable for structures used in harsh environments: high temperatures and pressures, corrosive environments, etc.

One of the recent application areas of the EXW technique is the bi-metallic parts of the Cern Compact Linear Collider (CLIC).[3]

Even though EXW has been used successfully for decades, many theoretical aspects of the process remain poorly understood. This is especially true for many microscopic details. These have been studied experimentally by observing the produced interface region using, e.g., electron microscopy. However, the collision *process* itself is a rapid and violent event making it obviously very difficult to observe in real time.

The collision in EXW—depending on the velocity and angle—produces a liquid jet at the point where the materials come to contact which is seen as essential for formation of a good bond. The jetting is believed to remove contamination layers on the surface of the metals allowing clean metal surface to come into contact. In addition to jetting, melting of thin layers of material near the interface is assumed to be a necessary condition for good bonding. Finally, the produced interface can exhibit a wavy character depending on the parameters of collision. The exact formation mechanisms of the interface waves is still under debate.

EXW process has been modeled with finite difference methods based on continuum description of materials.[4] These calculations need the constitutive equation of the material at high strains and strain rates and the equation of state of the explosive material as input. The jetting phenomenon has been reproduced using these methods.[5] However, it is not possible to model adhesion using continuum methods. The question whether the jetting correlates with the local transient melting of the interface region cannot be solved by continuum methods. Also, atomic level details of the bonding process are beyond reach.

In this study, we have simulated the EXW process with molecular dynamics (MD) method, which enables us to examine the process on the atomic level. The jetting phenomenon and interface melting were found to be

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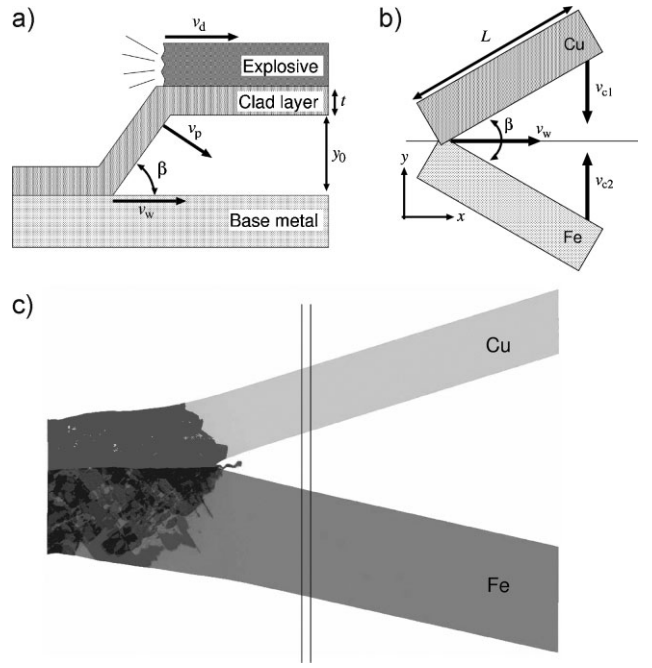

Fig. 1. (a)The principle of explosion welding. The clad layer with thickness t is initially at stand-off distance y_0 from the base metal. The detonation front advances with velocity v_d causing the clad layer to collide with velocity v_p and at angle β with the base metal. The welding point advances with velocity v_w. (b) Simulation setup. Metal slabs collide with velocities v_{c1} and v_{c2} and at angle β. The collision point advances with velocity v_w. (c) Snapshot of EXW simulation. Vertical lines show the position of the slice for which the temperature profile is depicted in Figure 4.

correlated, such that jetting is only observed when the interface melts. The interfacial wave formation and the peeling off of atomic layers from the bonding surfaces were also observed in the simulations. A nanocrystalline structure was observed near the interface after bonding process.

1. Simulation Method

The EXW process was simulated using the MD method.[6] In this method, equations of motion of an ensemble of atoms interacting via a force model are integrated numerically to follow the time development of an atomic system. The simulation results in detailed atomic level information of the dynamics of the system. Being a computationally heavy method, the time scale in MD simulations is restricted to no more than tens of nanoseconds and the system size up to 10^9 atoms. The MD method is widely used in materials research in studies where the atomic level modeling is needed.[7]

In this work, the code PARCAS[8,15,16] was used in the simulations. It has been previously used to model metal interfaces[9] and surfaces[10] and it has been optimized for large-scale parallel computations. The interaction model was an EAM-potential for Fe–Cu systems developed by Pasianot and Malerba to describe the thermodynamics of Fe–Cu alloys.[11] This potential also reproduced reasonable values for the Fe–Cu interface energy ($\gamma = 3.0 \pm 0.9\,\mathrm{J \cdot m^{-2}}$) as calculated for spherical α-Fe precipitates in Cu.

Table 1. Explosion welding simulations.

β [°]	v_c [km · s^{-1}]	Jet	Melting
15	1.5	No	No
15	2.0	No	No
20	1.5	Yes	Yes
25	2.0	Yes	Yes
30	1.0	Beginning	Yes
30	1.5	Yes	Yes

The simulation setup is show in Figure 1(b). Slabs of Fe and Cu collide with relative velocity (defined as $v_c = |\mathbf{v}_{c1}| + |\mathbf{v}_{c2}|$) of 1–2 km · s^{-1} at an oblique angle, as in typical experiments. The slabs were roughly 400 nm long and 50–100 nm thick. In the z-direction the system was very thin (roughly 4 nm) and periodic, mimicking an infinite system. The system contained roughly 20 000 000 atoms. The colliding surfaces were fcc (100) and bcc (100) for the Cu and Fe parts, respectively. All simulations were run until the Cu and Fe slabs were joined for their whole length. This was—depending on the collision angle and velocity—typically 70–120 picoseconds (ps). Table 1 lists the EXW parameters of simulations performed in this work.

Because Fe and Cu crystals have incommensurate unit cell sizes, the system size in the z-direction had to be chosen carefully so that the mismatch would not cause excessive stress in the slabs. One can fit 14 Fe unit cells and 11 Cu unit cells into the 4 nm thickness resulting in a mismatch of about 0.5%.

The initial temperature of the material was 0 K in earlier and 300 K in later simulations. The initial temperature was not observed to have a great effect on the outcome.

A few atomic layers at both ends of both slabs were fixed in the x-direction. In some earlier test simulations, in which the ends were not fixed, the whole system tended to stretch exceedingly in the x-direction sometimes almost breaking in half. The slabs used in the simulation are of course far thinner in the y-direction than in an actual macroscopic welding event and the presence of open boundaries above and below the weld line introduce distortion. The boundaries can, e.g., reflect the shock waves produced in the impact. To reduce these kind of effects absorbing boundary conditions were utilized. The boundary conditions consisted simply of a friction force applied to a layer of atoms close to the boundary. The force was proportional to the difference of the initial and current velocity. With a rough impedance matching the reflections are much weakened. The boundary conditions also act as a heat bath, cooling the system down. This mimics a larger system where the heat produced in the impact can be conducted away to more remote parts of the system.

2. Results

The simulations produced a welding process that was very similar to experiments. In particular, several simulations

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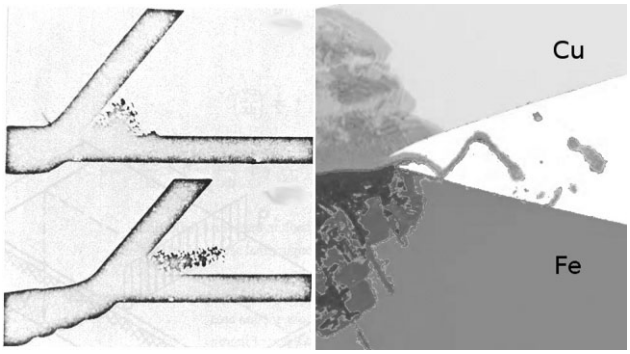

Fig. 2. On the left: flash X-ray images of jet formation in explosion welding. From Ref.[12] on the right: jet formation observed in the simulations. ($\beta = 30^\circ$, $v_c = 1.5\,km \cdot s^{-1}$).

reproduced the jetting phenomenon which is believed to be essential for forming a good bond. Whether jetting is observed or not was found to depend on the velocity and angle of impact. In some simulations a wavy interface was produced similar to what one often observes in actual welding. Figure 2 shows an example of a jet observed in the simulation along with flash X-ray images from experiments.

Analysis of the temperature distributions (Figure 3) showed that jet formation seemed to be connected to a rise of temperature beyond the melting point of the material. Jet formation always occurred only after sufficient a rise in temperature. This supports the conclusion that small localized melting is necessary for jet formation. This is well in line with experimental indications that melting of thin layers of material at the interface is necessary to reach bonding.[13] According to Figure 3, the melting lasts of the order of 100 ps.

We also examined which atoms are expelled in the jet. It appears that up to 20 or 30 topmost atomic layers (about 4 nm) are peeled off from copper and iron surfaces, respectively. The thickness of the peeled off layer tended to grow and in a larger simulation more atomic layers would have probably been removed. This kind of process would scour the surface clean of any oxides, although there was no actual oxide layer present in the simulation.

After the collision phase was completed the system was left in a nanocrystalline state with typical crystallite sizes of 10–20 nm. Figure 4 shows the simulation system after it has been cooled down to 0 K temperature in order to ease the structural analysis. In EXW the velocities of the slabs are so large that stresses at the collision point are much larger than the material strength, and severe plastic deformation occurs, producing nanocrystalline structure. Severe plastic deformation is actually utilized in producing nanocrystalline materials.[13]

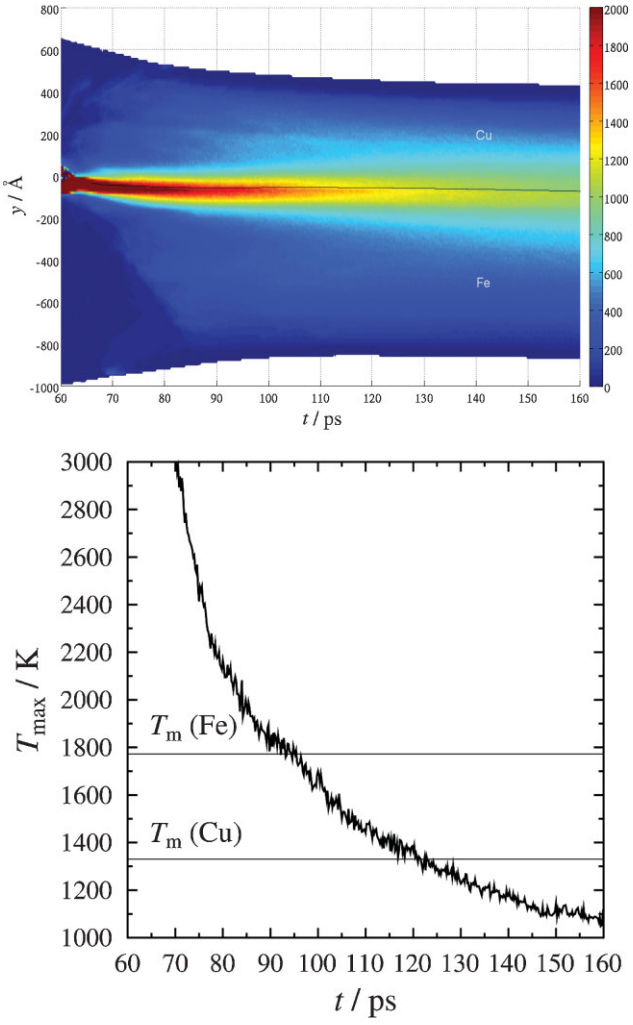

Fig. 3. Upper part: time development of the temperature profile along a vertical slice in the center of the simulation sample. Black line shows the position of the Cu–Fe interface. ($\beta = 30^\circ$, $v_c = 1.5\,km \cdot s^{-1}$). Lower part: maximum temperature in the system as a function of time. Horizontal lines show the melting temperatures of Fe (1772 K) and Cu (1330 K) predicted by the potential model used.[9] ($\beta = 30^\circ$, $v_c = 1.5\,km \cdot s^{-1}$).

with the same impact velocities and angles as in experiments. The results show jet formation, an increasingly fine grain size near the welded interface, and peeling off of the atom layers nearest to the interface, in agreement with experiments.

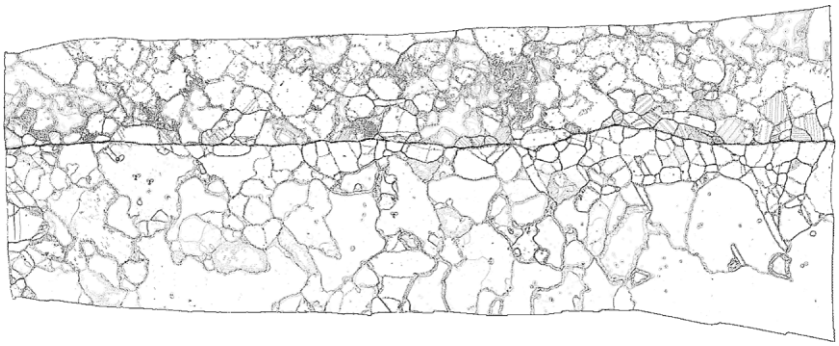

Fig. 4. Structure of the simulation system after welding and annealing. Darker regions show the boundaries nanocrystals and the thick dark line shows the position of the Cu–Fe interface. The system has been cooled to 0 K to make grains easy to separate. ($\beta = 30^\circ$, $v_c = 1.5\,km \cdot s^{-1}$).

3. Conclusions

We have simulated the EXW process on an atomic level using MD computer simulations

Analysis of the process further showed that a necessary and sufficient criterion for the jet formation is transient melting of material at the interface.

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[1] S. H. Carpenter, R. H. Wittman, *Annu. Rev. Mater. Sci.* **1975**, *5*, 177.
[2] N. V. Naumovich, A. I. Yadevich, N. M. Chigrinova, in *Shock Waves for Industrial Applications* (Ed: L. E. Murr) Noyes Publications, Park Ridge, New Jersey **1988**, Ch. 5, pp. 170–213.
[3] G. Arnau-Izquierdo, S. Calatroni, S. Heikkinen, T. Ramsvik, S. Sgobba, M. Taborelli, W. Wuensch, *IEEE Part. Accel. Conf.* **2007**, *1–11*, 3953.
[4] A. A. Akbari Mousavi, S. J. Burley, S. T. S. Al-Hassani, *Int. J. Impact Eng.* **2005**, *31*, 719.
[5] A. A. Akbari Mousavi, S. Al-Hassani, *J. Mech. Phys. Solids* **2005**, *53*, 2501.
[6] D. Frenkel, B. Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, Vol. *1* of Computational Science Series, 2 Edn., Academic Press, San Diego **2002**.
[7] S. Yip Ed., *Handbook of Materials Modeling*, Springer, Germany **2005**, Part A, Ch. 2.
[8] K. Nordlund, **2006**, PARCAS computer code. The main principles of the molecular dynamics algorithms are presented in [15, 16].
[9] K. Nordlund, R. S. Averback, *Phys. Rev. B* **1999**, *59*, 20.
[10] K. Nordlund, J. Keinonen, M. Ghaly, R. S. Averback, *Nature* **1999**, *398*, 49.
[11] R. Pasianot, L. Malerba, *J. Nucl. Mater.* **2007**, *360*, 118.
[12] V. V. Kuznetzov, *Phase Transformation Effects Under High Dense Energy on Matter* Novosibirsk Academy of Science, Siberian Branch, Novosibirsk, USSR **1985**.
[13] M. Nishida, A. Chiba, Y. Honda, J. Hirazimi, K. Horikiri, *ISIJ Int.* **1995**, *35*, 217.
[14] R. Valiev, *Nat. Mater.* **2004**, *3*, 511.
[15] K. Nordlund, M. Ghaly, R. S. Averback, M. Caturla, T. Diaz de la Rubia, J. Tarus, *Phys. Rev. B* **1998**, *57*, 7556.
[16] M. Ghaly, K. Nordlund, R. S. Averback, *Philos. Mag. A* **1999**, *79*, 795.

