Molecular Dynamics Simulation of Copper-Niobium Interfaces

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INTRODUCTION

- Copper-niobium composites were developed and used in high field magnets because of their high mechanical strength and low electrical resistivity; Cu-Nb interfaces influence both properties.[1]
- During the fabrication, e.g. heat treatment, of Cu-Nb composites, interface reactions may occur. We studied the Cu-Nb interface in both Cu-2.6 wt %Nb and Cu-9.5 wt %Nb composites using Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).[2]
- LAMMPS is a Molecular Dynamics (MD) code developed by Sandia National Labs. MD is a computer simulation method to study atoms and molecules and utilizes interatomic potentials and Newton's equations of motion to calculate atomic forces and atom trajectories. MD can be used to simulate equilibration and tension in materials, and to study defects.[3]

PROCEDURE

- LAMMPS input scripts for the respective systems were written and executed in the terminal of an Ubuntu Linux computer. The EAM FS potential used was derived by Gong *et al*.[4] and made LAMMPS compatible using a python package, atsim.potentials, developed by Rushton.[5] The CuNb composites were oriented so that $[1\ 1\ 1]_{Cu} \| [1\ 1\ 0]_{Nb}$ and $[1\ \bar{1}\ 0]_{Cu} \| [\bar{1}\ 1\ 1]_{Nb}$. Both systems were minimized and then equilibrated for 500 ps with no external forces at 300 K and 800 K. CFG files were generated for each simulation and used for visualization in AtomEye[6] and OVITO[7].

RESULTS AND DISCUSSION

- For particle and fiber shaped Nb embedded in Cu matrix, increasing the temperature led to increased instability of the Cu-Nb interface. Atoms at the interface exhibited higher coordination numbers and solid dissolution occurred.
- At 300 K, after 500 ps, majority of the copper and niobium atoms retained their respective FCC and BCC lattice structures.
- At 800 K, majority of the niobium atoms failed to retain a BCC lattice structure.
- In the Cu-2.6 wt %Nb composite, which has more Cu-Nb interfaces compared to the Cu-9.6 wt %Nb composite, vacancies formed along the interface as the system was brought to equilibrium.
- To minimize interface energy, it was expected that the Cu-Nb interfaces would align to a particular interface orientation, but such was not observed. This may be related to the small size of the Nb in the system.

Copper-niobium interfaces **lose structure** and become **increasingly unstable** as the temperature of the system **rises**.

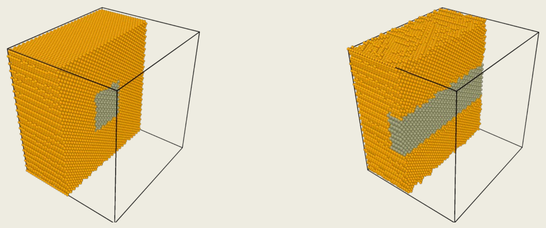

Figure 1. Sectioned Cu-2.6 wt %Nb (left) and Cu-9.5 wt %Nb (right) simulation cells. In Cu-2.6 wt %Nb , a Nb particle with dimensions of 1.8 nm x 1.8 nm x 1.8 nm embedded in Cu. In Cu-9.5 wt %Nb , a Nb fiber with dimensions of 1.8 nm x 7.2 nm x 1.8 nm embedded in Cu.

FUTURE WORK

- The study can be extended to model the Cu-Nb interfaces under uniaxial tension at both 300 K and 800 K.
- The study can be made more realistic by increasing the size of the simulation cell and introducing more niobium particles and fibers in the respective simulations.

ACKNOWLEDGEMENTS

This research was funded by NSF grant DMR 1644779. Many thanks to Mark Tschopp[8] for LAMMPS Tutorials.

REFERENCES

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ADDITIONAL RESULTS

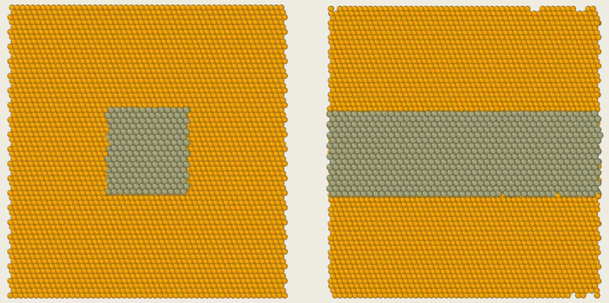

Figure 2. Cross-sections of the Cu-2.6 wt %Nb (left) and Cu-9.5 wt %Nb (right) simulation cells at 0 K. Most of atoms remain at their original FCC and BCC structure with coordination numbers between 5 and 14.

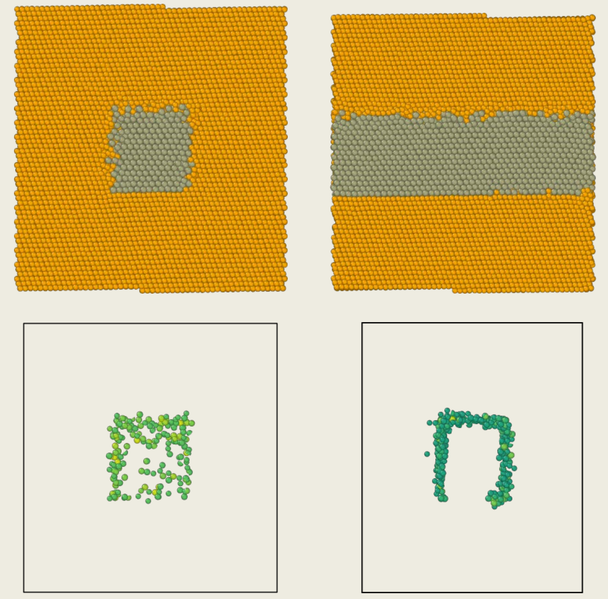

Figure 3. Cross-sections of the Cu-2.6 wt %Nb (top left) and Cu-9.5 wt %Nb (top right) simulation cells at 300 K after equilibration for 500 ps. Atoms with a coordination number greater than 15 are shown for Cu-2.6 wt %Nb (bottom left) and Cu-9.5 wt %Nb (bottom right); the brighter the color, the higher the coordination number.

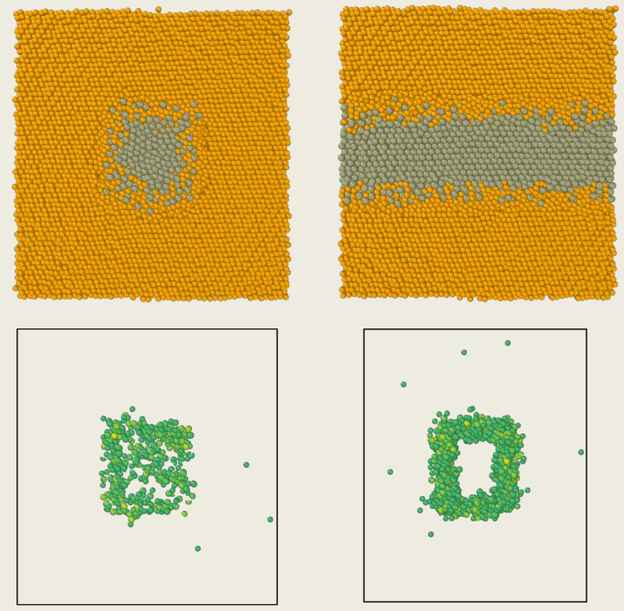

Figure 4. Cross-sections of the Cu-2.6 wt %Nb (top left) and Cu-9.5 wt %Nb (top right) simulation cells at 800 K after equilibration for 500 ps. Atoms with a coordination number greater than 15 are shown for Cu-2.6 wt %Nb (botton left) and Cu-9.5 wt %Nb (bottom right); the brighter the color, the higher the coordination number. Some Nb atoms diffused to Cu matrix.