

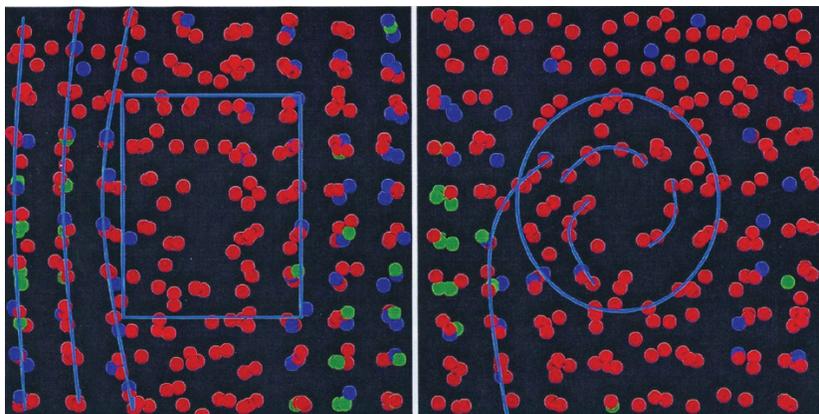
Molecular Dynamics Simulations of Shock-Induced Microstructure Evolution and Helium Bubble Diffusion in Metals

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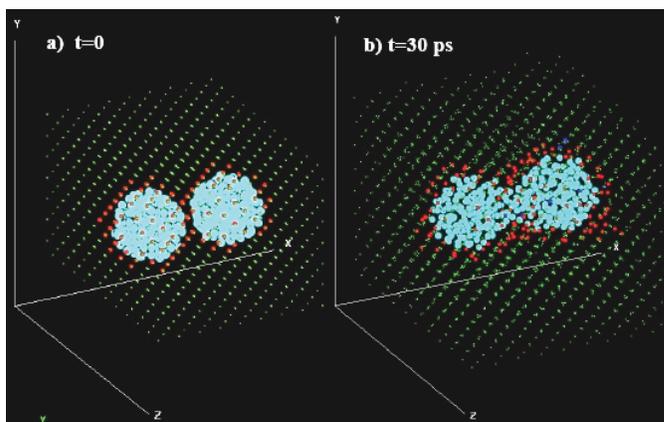
Project Description

The development of physically based mathematical models capable of predicting material response to arbitrary thermomechanical loading requires, in general, an understanding of physical mechanisms at multiple length scales. However, experimental capabilities for probing atomistic length scales under dynamic conditions are extremely limited. It is the goal of this project to compensate for this shortcoming in current experimental capabilities by carrying out a suite of molecular dynamics simulations to obtain numerical approximation of microstructural changes that take place in metals because of shock wave loading, and to investigate a number of issues related to the aging of plutonium.

With respect to microstructural changes that take place in metals due to shock wave loading, a number of issues are to be investigated. Examples include a determination of (1) the dominant mechanism for stress relaxation in polynanocrystalline metals and (2) the fundamental mechanisms involved in the initiation and evolution of damage in monocrystalline and polynanocrystalline metals. Preliminary results reveal that the dominant mechanism for stress relaxation in polynanocrystalline metals is through the



Damage initiation showing vortical atomic motion resulting in an approximately spherical void. (Phys. Rev. B, V74, No. 14, p144110)



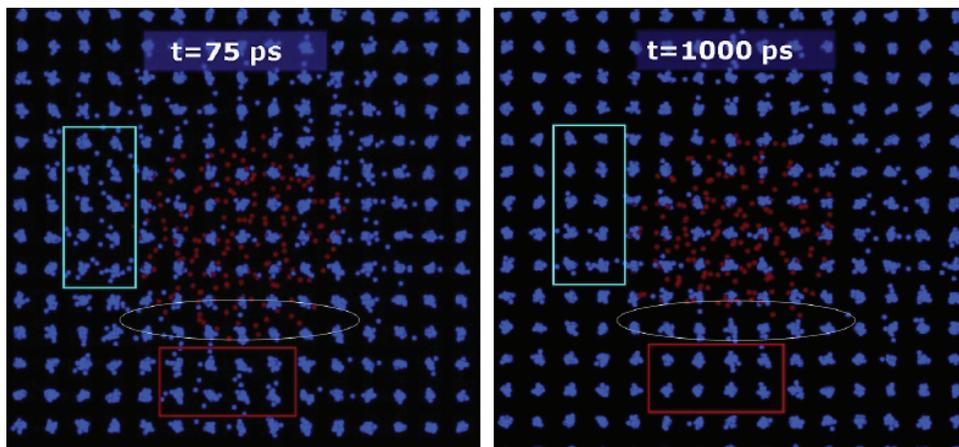
Simulation of bubble-bubble interaction.

production of stacking faults. Results obtained thus far on the initiation of damage reveal a tendency for damage to initiate in regions where stacking fault densities are high, especially at stacking fault intersections. Damage initiation is observed to proceed from the breaking of the first molecular bond to the formation of approximately spherical voids in a time span on the order of 0.2 ps. Vortical atomic motion, resulting in approximately spherical voids, is observed even in cases where the loading is approximately uniaxial.

One of the consequences of the aging of plutonium is an ever-increasing presence of helium trapped within the plutonium lattice. In order to predict the long-term effects of this, it is imperative that we gain a better understanding of the fundamental mechanisms involved in He-Pu interactions and the resultant effects of these interactions on macroscopic response. Issues to be investigated include the diffusion of He in a Pu lattice, He bubble formation, bubble-bubble interaction, the mechanics of self-irradiation damage in Pu already containing He bubbles, and He bubble diffusion.

Technical Purpose and Benefits

Much remains to be learned concerning the fundamental mechanisms that govern material constitutive response and the initiation and evolution of damage. This work supports the goals of the NNSA and the research institutions (LANL and VNIITF) for the development of more physically based mathematical models, models that are truer to the fundamental physical mechanisms at play, and models that account for more of the physics. Gaining a better understanding of the fundamental mechanisms involved in the aging of plutonium and in the consequences of that aging on the macroscopic response of the material is critical for LANL to meet its responsibilities to the NNSA and the country. This work supports the objectives of the NNSA and both research institutions (LANL and VNIITF) as they endeavor to improve their predictive capabilities with respect to plutonium aging and the consequences thereof.



Pu lattice in the vicinity of a He bubble (He to vacancy ratio 3:1; $T = 600$ K) at two different times – Pu atoms in blue; He atoms in red.

Collaboration between Los Alamos National Laboratory, Los Alamos, NM, USA, and the Russian Federal Nuclear Center – All Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, Russia

