STRONGLY NON-ARRHENIUS INTERSTITIAL DIFFUSION IN VANADIUM--L. A. Zepeda-Ruiz (Lawrence Livermore National Laboratory), S. Han (Princeton University), G. J. Ackland (University of Edinburgh), R. Car (Princeton University), and D. J. Srolovitz (Princeton University),

ABSTRACT

The creation and evolution of point defects play an important role in determining the structural properties of materials. The two elementary point defects in elemental metals are vacancies and self-interstitial atoms (SIA). The creation and migration of SIA are critical for microstructural evolution of materials in high-energy radiation environments and in ion implantation. SIAs are usually very mobile (i.e., the migration barriers for SIAs are relatively small) and, hence, play an important role in controlling the rates of several types of microstructural processes in such applications.

In this study, we examined the fundamental behavior of SIAs in vanadium through a series of molecular dynamics (MD) simulations based on an interatomic potential that is consistent with first principles calculations of point defects in V. We found that the stable SIA structure in V is a <111>-oriented dumbbell, rather than the <110>-oriented dumbbell found in Fe. Given this fundamental discrepancy, SIA migration in Fe and V must be fundamentally different and our current understanding of SIA diffusion in V is rather limited. In particular, we examined SIA diffusion as a function of temperature and determine the mechanisms that control it. We found that while SIA migration in V is similar to that in bcc Fe in many respects, several important differences exist and a range of interesting phenomena are observed.

Our MD results showed that <111>-oriented dumbells migrate quickly along <111> directions, even at very low temperatures. Rotation of the dumbbells and the migration path to other <111>-directions occurs with increasing frequency as the temperature is raised. The interstitial migration mechanism was found to be temperature dependent. For low and intermediate temperatures (100-600 K) the SIA executed an essentially one-dimensional (1D) random walk along a <111>-direction. Only 1D random walks were observed for temperatures from 100K to 600K. Upon increasing the temperature to T~700K, the SIA began to make infrequent rotations from one <111>- to another <111>-direction. This resulted in a 3D trajectory that consists of long 1D random walk segments with abrupt reorientations. As the temperature increased, the frequency of the rotation events increased and the lengths of the 1D segments of the trajectories decreased. At high temperatures, the rotation events became very frequent, such that the SIA is performing a truly 3D random walk. It was found that the apparent activation energy for diffusion increases with increasing temperature. This increase in apparent activation energy with increasing temperature occurs even at temperatures that are too low to be attributed to dumbbell rotation. Rather, we demonstrated that the intrinsic activation energy is not strongly temperature dependent, but rather the correlation factor is.

REFERENCE

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