Euroopa Liit
Euroopa Sotsiaalfond

Eesti tuleviku heaks

Toetab TÜ ja TTÜ doktorikool “Funktsionaalsed materjalid ja tehnoloogiad”(FMTDK)

ESF projekt 1.2.0401.09-0079

STATE OF NIOBIUM EMPIRICAL POTENTIALS FOR RADIATION DAMAGE STUDIES

Artur Tamm, Alvo Aabloo

IMS Lab, Institute of Technology, Tartu University, Estonia

Modern nuclear reactors require materials that can withstand large doses of radiation for a long period of time. Nanoscale metallic multilayer composites like CuNb system (figure 1) have shown an improved radiation damage tolerance in comparison with bulk Cu and Nb. Large metallic interfaces in these materials act as absorbing sinks for defects, and in these regions material heals itself through recombination of interstitials and vacancies. Experimental study of such systems is timeconsuming and difficult, therefore multiscale simulation methods have to be applied in order to evaluate the usage of multilayer composites. Empirical potentials used in these studies have to be correct in regions where they were not fitted, thus some validation has to be made before they can be used.

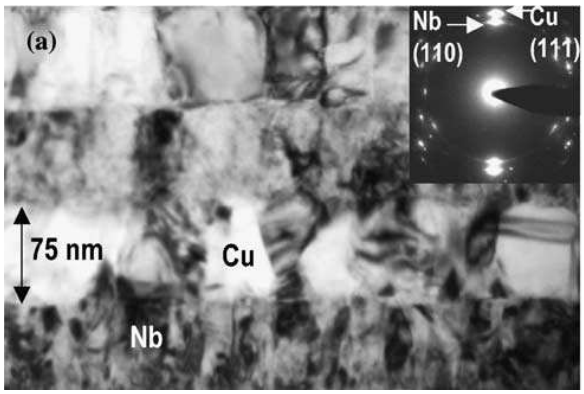

Figure 1: TEM picure of a CuNb multilayered material [1]

In this study we use DFT calculation results as comparison data in order to check the usability of empirical potentials. We calculated the cohesive energies of bulk niobium at different lattice constants. Energies for four crystal configurations were found (BCC, FCC, HCP, SC). In addition vacancy energies, selfinterstitial energies and elastic constants were calculated.

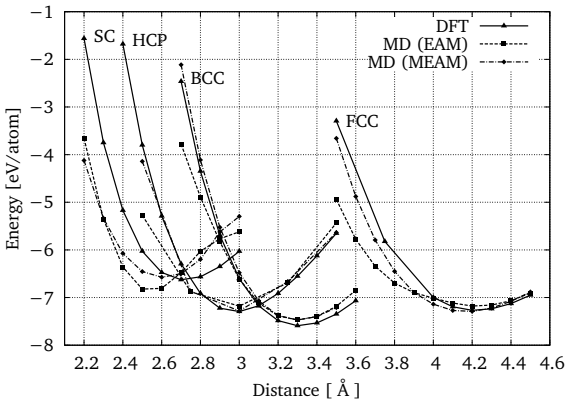

Figure 2: Cohesive energies of niobium crystal configurations

Two empirical potentials were chosen as candidates for niobium material. An EAM potential created by Demkowicz [2] and an MEAM potential by Lee [3], were chosen as the best currently available potentials. We repeated all the calculations done with DFT using the above mentioned potentials in an MD simulation, and the results are plotted on figure 2.

The results clearly show that the empirical potential fail to reproduce precisely DFT results, especially on low atomic distances, which might suggest, that in order to use them in radiation damage studies they should be improved.

References

[1] Mara, N., Sergueeva, A., Misra, A., and Mukherjee, A. K. *Scripta Materiala* **50**, 803–806 (2004).

[2] Demkowicz, M. J. and Hoagland, R. G. *International Journal of Applied Mechanics* **1**, 421–442 (2009).

[3] Byeong-Joo, L., Baskes, M. I., Hanchul, K., and Yang, C. K. *Physical Review B* **64**, 184102–1–184102–11 (2001).

Email address: arturt@ut.ee (Artur Tamm)