3 - 15 Resistance of Nano-scale Cu/Fe Interface to Radiation Damage Studied by Molecular Dynamics Simulations

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Iron-copper (Fe-Cu) alloy systems have been found with a variety of industrial applications from magnetic devices to nuclear reactor structural materials which leads to the wide investigations for these systems, especially in the form of multilayer thin film and alloys. Generally, the metallic multilayer has been known to have the unique properties for many years, especially in the applications of its mechanical, magnetic, thermal and optical properties. The metallic multilayer system with layer thickness of a few nanometer can reach the ultra high strength up to 1/3～1/2 of the theoretical value. Considering local structures of grain boundary and metallic multilayer interface, in this paper, the Fe-Cu multilayer systems have been studied focusing on the interface properties related with the binding of interstitials and the annihilation of vacancies by the interface in order to understand the ability of such interface to radiation damage.

As example, three different types of interfaces formed by Fe/Cu were chosen for further displacement cascade simulation. After full simulations, three different ways have been identified for interface to annihilate the formed vacancies in the interface range: ring-replacement, displacement replacement and direct-recoil.

After the cascade simulations, the stress-strain curve has been also calculated and compared with the case before these simulations. The results indicate that such interface has little effect on mechanical properties of system which indicates its resistance to radiation damage.

The interface mixing has been also observed after the cascade even the solubility of Cu in Fe is very low. Thus, the high energy implantation leads the mixing of the sharp interface, which may results in the new properties.

In summary, different nano-scale multilayer systems formed by Cu{hkl}/Fe{HKL} layers have been simulated with the recently developed Fe-Cu empirical potential. The local structure of interface shows different features after full relaxation. High positive binding energies of interstitial Fe or Cu to these interfaces have been found which indicates the strong absorption of interface to these defects. The displacement cascade simulations have been also performed and three ways have been found for these interface to annihilate the nearby left vacancy sites. Except the emission of Cu atom to vacancy sites, an exchange-ring has been also observed to annihilate the vacancy. The high tensile stress of Cu atoms could also induce the high energy PKA to return the original sites leading no damage left. After 50 displacement cascade simulations, the semi-coherent interface decrease the stress because of the more left defects in the interface while the stress-strain curve has only slight change for incoherent interfaces. With high PKA energy, the displacement cascade can also lead to the intermixing of Fe/Cu layer although very low solubility of Fe in Cu.