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Editorial

Numerical Modeling of Materials under Extreme Conditions

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1. Introduction and Scope

Materials used under extreme conditions are important in various industrial and defense fields [1,2]. The performance of these materials critically affects the lifetime of related facilities [1,2]. Thus, it is essential to explore the underlying damage mechanisms of materials under extreme conditions. Considering the difficulty and high cost of the experiments carried out to investigate these mechanisms, numerical modeling of the material response is crucial for study in these fields [3,4]. Until now, although various approaches and models from the atomic scale to the macroscale have been used or developed to simulate the mechanical response and microstructural evolution during the processes [4–8], detailed investigations are still needed to further understand the materials under extreme conditions.

The scope of this Special Issue embraces numerical work on material responses to extreme conditions such as high-speed impact or loading, neutron or ion irradiation, and high-pressure and/or high-temperature environment. Related simulation results based on the first-principle molecular dynamics and finite element methods are reported.

2. Contributions

The Special Issue collects contributions from different research groups by focusing on materials under extreme conditions, at various levels, with different simulation methods. Twelve papers, including eleven research papers and one review paper, have been reviewed and accepted by this Special Issue [9–20].

Ouyang et al. [9] fitted a new angular-dependent potential for a U-Mo system, which well reproduces the macroscopic properties of the system. The threshold displacement energy surface at intermediate and short atomic distances is also more accurately described by this new potential. Furthermore, simulations based on this potential corroborate the negative role of local Mo depletion in the mitigation of irradiation damage and consequent swelling behavior.

Zeng et al. [10] simulated the adsorption and diffusion behaviors of a Na atom on a Mo (110) surface with the presence of Re and O atoms by the first-principles approach. The result shows that the Re alloy atom can strengthen the attractive interactions between Na/O and the Mo substrate, and the existence of a Na or O atom on the Mo surface can slow the Na diffusion by increasing the diffusion barrier. The surface vacancy formation energy results indicate that the dissolution of Mo is a potential corrosion mechanism in the liquid Na environment with O impurities. Furthermore, Liu et al. [11] performed ab initio molecular dynamics simulations to understand the interactions between the Na solvent and Mo or Re solute in the liquid phase. It was found that Mo_2 and Re_2 dimers can be stabilized in liquid Na and a higher temperature leads to a stronger binding force. The Mo species diffuse faster than the Re species and the diffusivity decreases as the cluster size increases.

Li et al. [12] employed molecular static simulations to investigate the interaction between a 1/2 [111] interstitial or vacancy dislocation loop and a vacancy-type defect

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including a vacancy, di-vacancy, and vacancy cluster in tungsten (W), through binding energy calculations. Furthermore, the effect of a vacancy cluster on the mobility of the 1/2 [111] interstitial dislocation loop was also explored by the molecular dynamics method. The results indicate that a vacancy cluster can attract the 1/2 [111] interstitial dislocation loop and pin it at low temperatures. At high temperatures, the 1/2 [111] interstitial dislocation loop can move randomly.

Using molecular dynamics methods, Dai et al. [13] calculated the elastic constants C_{11}, C_{12}, C_{44}, bulk modulus, and shear modulus of FeCrAl alloy, one of the candidate materials for accident-tolerant fuel (ATF) cladding in the nuclear power industry. The results show that the concentrations of Al and Cr have different effects on the elastic constants. When the concentration of Al was fixed, a decrease in bulk modulus and shear modulus with increasing Cr content was observed, which is consistent with previous experimental results. The dependence of elastic constants on temperature was also the same as in the experiments. Investigations into the elastic properties of defect-containing alloys have shown that vacancies, void, interstitials, and Cr-rich precipitations have different effects on the elastic properties of FeCrAl alloys.

Wang et al. [14] investigated the influence of radiation defects on the thermo-mechanical properties of UO_2 within 600–1500 K through the molecular dynamics method. The results indicate that these point defects reduce the thermal expansion coefficient (α) at all studied temperatures. The elastic modulus at finite temperatures decreases linearly with an increase in the concentration of Frenkel defects and antisites. All these results indicate that Frenkel pairs and antisite defects could degrade the performance of UO_2.

Xia et al. [15] simulated the behavior of xenon (Xe) bubbles in uranium dioxide (UO_2) grain boundaries by using the molecular dynamics method. The results indicate that the formation energy of Xe clusters at the Σ5 grain boundaries (GBs) is much lower than in the bulk. The diffusion activation energy of a single interstitial Xe atom at the GBs was approximately 1 eV, lower than that in the bulk. The bubble pressure dropped with increasing temperature at low Xe concentrations, whereas the volume increased. Xe atoms were more regular in the bulk, whereas multiple Xe atoms formed a planar structure at the GBs.

Wang et al. [16] studied the effects of point defects on the behaviors of Xe/Kr clusters in UO_2 by using molecular dynamics. The results show that Xe and Kr clusters occupy vacancies as nucleation points by squeezing U atoms out of the lattice, and the existence of vacancies increases the stability of the clusters. Higher temperature and higher concentrations of interstitial Xe/Kr atoms or vacancies in the system all facilitate the formation of the clusters. The activation energy of interstitial Xe/Kr atoms and clusters in UO_2 is ~2 eV, indicating that the diffusion of the interstitial atoms is very difficult.

Xiao et al. [17] simulated the influence of grain boundaries on Fe-H_2O interfacial corrosion through the molecular dynamics method with a new Fe-H_2O reaction force field potential. The results indicate that the corrosion rate at the polycrystalline grain boundary is significantly higher than that of twin crystals and single crystals. By the analysis of stress, it can be found that the stress at the polycrystalline grain boundary and the Σ5 twin grain boundary decreases sharply during the corrosion process. The severe stress release at the grain boundary could promote the dissolution of Fe atoms. The formation of vacancies on the Fe matrix surface will accelerate the diffusion of oxygen atoms, resulting in the occurrence of intergranular corrosion.

Ma et al. [18] investigated the evolution of atomic structures and related changes in the energy state, atomic displacement, and free volume of several symmetrical grain boundaries (GB) under the effects of external strain in body-centered cubic (bcc) iron by the molecular dynamics (MD) method. The results indicate that under external strain, two mechanisms are responsible for the failure of these GBs, including slip system activation, dislocation nucleation, and dislocation network formation. This is induced directly by either the external strain field or by phase transformation from the initial bcc to fcc structure under the effects of external strain.

Lee et al. [19] performed a side crash simulation and investigated the effect of hot press forming (HPF) a center pillar with a combination of patchwork (PW) and partial softening (PS) techniques on collision toughness and energy distribution flow. The roles of the PW and PS techniques were verified during the side crashes. PW improves the strain energy and intrusion displacement by 10% and 7.5%, respectively, and PS improves the plastic deformation energy and intrusion displacement by 10%. When PW and PS were applied to the HPF center pillar simultaneously, a synergistic effect was achieved.

Wang et al. [20] reviewed the experiments and models for the effect of strain rate on NiTi shape memory alloys (SMAs). Experimental observations on the rate-dependent properties, such as stress responses, temperature evolutions, and phase nucleation and propagation, under uniaxial loads, are classified and summarized based on the order of the strain rate magnitudes, with the influences of the microstructure on the strain-rate responses briefly discussed. This review of modeling for the rate-dependent behaviors of NiTi SMAs focuses on how the physical origins are reflected or realized in the constitutive relationship.

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