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The shock response of crystalline Ni with H-free and H-segregated ⟨1 1 0⟩ symmetric tilt GBs

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ABSTRACT

The shock responses of crystalline Ni with two types of symmetric tilt grain boundaries (STGBs) are studied by large-scale molecular dynamics simulations, with special concerns on the effect of hydrogen segregated STGBs on them. The crystalline Ni with different kinds of H-free STGBs have significantly different plastic responses during the shock processes due to different mechanisms of dislocation emission from the STGBs. The segregation of hydrogen atoms at the STGBs significantly affects the dislocation emission from the H-segregated STGBs, and then heavily affects the shock plastic responses of crystalline Ni with H-segregated STGBs. On the one hand, dislocation emission from the H-segregated STGBs is delayed compared with that from the H-free ones at the low shock velocity, showing the so-called lagging effect. On the other hand, multi-mode dislocation emissions (or dislocation emission on the multi slip systems) are frequently activated from the H-segregated STGBs at the high shock velocity. In addition, the spallation behavior of the crystalline Ni under shock loading is also significantly affected by hydrogen segregation at the STGBs. In the targets with the H-free STGBs, spallation originates mainly from the interior of the grains due to strong interaction and reaction between dislocations there, however, it originates definitely from the H-segregated STGBs due to the reduced GB cohesive strength by hydrogen segregation.

1. Introduction

It has been long recognized the internal microstructures of materials strongly dominate their macroscopic mechanical behaviors [1–5]. Guided by this, materials scientists have designed or synthesized various architectural nano/micro-structured materials, such as materials embedded with nano-twinned [1,3], gradient [2], hierarchical [4,6] or laminated [5,7] structures, aiming at improving their strength and ductility to cope with harsh and extreme environment. In addition to the internal microstructure design, another way to promote the mechanical properties of metallic materials is the alloying strategy with certain solute elements [8–13]. As a matter of fact, alloying elements can not only influence the characteristic microstructure but also the plastic deformation mechanisms [12], bringing about kinds of strengthening mechanisms and high/low-temperature stability [9]. In certain scenario, a small amount of solutes can drastically affect the global materials properties, rendering extraordinary strength and ductility [8,10,14]. Nevertheless, some special solutes which are unavoidably introduced from the commercial process or service environment are deleterious to the material, such as O, N, H and so on [10], especially when these impurities segregate at grain boundaries (GBs) or other defective structures. The internal microstructures as well as the alloying or impure solutes are important to the mechanical response of metallic materials, which can synergistically determine their service reliability under impulsive load.

Nowadays, with the development of advanced technology, the shock response of nano/micro-structured materials becomes an increasingly significant scientific problem in laser processing [15], explosion impact [16], nuclear fusion reactors [17] and other critical conditions. Some researches have indicated that different microstructures such as polycrystalline structure, twinned structure and multilayered structure could certainly result in different shock responses [7,18–20]. It must also be mentioned that these ensemble microstructures are such complicated that their exact shock response can't be deeply understood. As shown in some researches, slight difference of GBs can be recognized by the shock

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wave and thus affect heavily the shock response [21]. Therefore, it is necessary to study more fundamentally the shock response of the microstructure.

As we know, the importance of solute segregation to the static or quasi-static mechanical behaviors of materials has been widely recognized [10,14], but there are relatively few studies devoted to its effect on the shock response of materials. In this paper, the effect of a usual solute segregation, i.e. hydrogen segregation, on the shock response is discussed to gain a primary insight on it. In many engineering fields, such as the fusion reactor, the plasma facing components not only sustain the thermal and mechanical shock, but also bear the threat of waste hydrogen and its isotope. The retention of hydrogen can degrade the mechanical property of metals [22,23] and cause unforeseeable catastrophe, which is known as the hydrogen embrittlement (HE). The intractable HE problem is becoming a challenge with increasing utilization of hydrogen energy. As the smallest atoms, hydrogen atoms can enter easily the metallic metals, then diffuse fast in metallic lattice until they are trapped by various defects in metals [24], such as grain boundary. The hydrogen segregation at GBs plays an important role in the interaction between the dislocation and the GB as well as the slip transfer of dislocations across the GBs [25], which finally leads to the intergranular failure [23]. On the other hand, hydrogen segregation at GBs may also significantly affect plastic deformation mechanisms, such as GB sliding, GB migration, twinning, and dislocation emission process [13,26]. Although there are many studies on how the solute hydrogen significantly affects the strength, plasticity and fracture of metals serviced in hydrogen environment, seldom work was done to study its effect on the deformation behavior and its mechanism of materials subjected to a shock loading. Previous research showed that the solute hydrogen could facilitate the multiplication of both dislocations and vacancies, resulting in high defect density in palladium under shock condition [27]. Nevertheless, how the solute hydrogen segregated at GBs affects the shock response is still indistinct. In this paper, we will pay a special attention to the effect of solute hydrogen segregated at the GBs on the shock response, especially on the plastic and spall behaviors.

As we know, under femtosecond laser impact or explosion, where the ultra-high strain rate is on the order of $10^6 \sim 10^9$/s and the ultra-short acting time is on the order of $10^{-12} \sim 10^{-9}$ s [28], the ultra-fast evolution of microstructures can hardly be captured in normal conditions, which brings much difficulty to implementation of tests and subsequent data collection. On the other hand, the experimental tests under extreme conditions usually are extremely expensive. For these, numerical modeling method becomes crucial in shock researches. To respond to the high/ultra-high strain rate in impact or shock condition, discrete dislocation dynamics (DDD) [29–32] and molecular dynamics (MD) [33–37] are the most optimal computing technology, due to their inherent high/ultra-high strain rate capacity. Compared with DDD modeling, MD modeling can achieve even higher strain rate. More importantly, MD are more physical which can directly capture the atom details and visually reveal the fundamental mechanism if a sufficiently accurate potential is adopted. As a matter of fact, MD comes of age for shock wave research [38] and is becoming a powerful computational tool to capture the shock response of materials. In the past few decades, a large number of MD simulations have been successfully implemented to study the effect of shock wave on the plastic and spall behaviors in single crystalline [39–41], bi-crystal [42,43], polycrystal [44], and thermal shock in femtosecond pulse laser process technology [37], trying to expose the underlying deformation and failure mechanisms.

Motivated by the above background and considering the advantage of the MD method in the shock study, we adopt the MD modeling to study the shock response of one kind of simple GB, i.e. symmetric tilt grain boundary (STGB), with special concern on the plastic and spall behaviors. At the same time, hydrogen segregation at the STGB also is considered to shed light upon its effect on the plastic and spall behaviors under shock loading. The paper is organized as follow: Section 2 addresses the setup of the hydrogen segregated STGBs and shock models, as well as methodology for MD simulations. Section 3 presents the results and discussions. And at last, the paper is ended with some main conclusions in Section 4.

2. Model and methodology

To facilitate the result analysis, the STGB in Ni with a tilt axis $\langle 1\ \bar{1}\ 0\rangle$ is selected to investigate its shock response. Two typical $\Sigma 9(114)$ and $\Sigma 33(441)$ STGBs, which are of low (38.94°) and high (159.95°) misorientation angles, are considered, respectively. The grain orientation relationships on both sides of $\Sigma 9(114)$ and $\Sigma 33(441)$ STGB are shown in Fig. 1(a) and (b), respectively. The STGBs are constructed according to Tschopp et al.'s strategy [45,46]: By means of rigid body translations between two neighboring grains and the deletion of overlapped atoms with a proper distance criteria followed by the energy minimization of the whole system, the finial GB configuration with the lowest average energy is selected as the objective STGB model, as shown in Fig. 1(a) and (b), respectively. The obtained $\Sigma 9(114)$ and $\Sigma 33(441)$ STGB structures are checked through structural unit model (SUM), which are the same as ones in the previous STGB study [47]. After the objective STGB models are settled down, H atoms are introduced into the model through an equilibrium segregation model which has been extensively used in the H-segregation modeling [25,48,49]. The readers are suggested to refer to [49] for more details of the implementation scheme. Using the above-mentioned model, H atoms are segregated mainly at STGB where there is high binding energy. The finial hydrogen segregations at $\Sigma 9(114)$ and $\Sigma 33(441)$ STGBs are shown in Fig. 1(a) and (b) in which H atoms are represented by the green[1] particles. To validate the reliability of this segregation model, the Monte Carlo (MC) method also is employed to relax the H-segregated STGB. The result shows the systemic energy keeps almost constant during MC modeling process, which implies the hydrogen segregated STGB configurations are energetically stable. To make a preliminary acquaintance of the hydrogen effect on the dislocation emission strength and mechanism which are essential to understand the plastic behavior of pure/impure STGBs under shock loading, the uniaxial tension and compression of the H-free and H-segregated bi-crystals Ni are studied beforehand. These results are given below in Section 3.1.

With the H-free/segregated STGBs, we construct the flyer plate-target shock model which is illustrated in Fig. 1(c). The shock direction is along the Z-axis which is perpendicular to the STGBs. The spacing between STGBs is defined as L. In order to study the effect of STGB spacing (or grain size) on the shock response, L is assigned as 10, 20, and 40 nm, respectively. The cross-sectional areas are equal for both the flyer plate and the target, while the length of flyer plate is one half of the target in the shock direction to reduce the computation cost. The periodic boundary conditions are exerted in both the X and Y directions which are transverse to the shock direction. The entire computational model is approximately 20 nm × 20 nm × 120 nm, containing more than 3.8 million atoms. Our computation shows that a larger MD model generates a consistent result with the present model. After the shock model is setup, the system is first relaxed via energy mini-

[1] For interpretation of color in Figs. 1 and 3, the reader is referred to the web version of this article.