Simulation Study on Mechanical Properties of Defective Titanium Metal (Postprint)

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Date: 2023-03-19T00:00:00+00:00

Abstract

Using molecular dynamics simulation methods, the effects of vacancies, self-interstitial impurity atoms, impurity He atoms, and other defects on the mechanical properties of metallic Ti samples were investigated respectively. Stress-strain curves for perfect lattice metallic Ti at different tensile strain rates were calculated, and it was found that the tensile process can be divided into three stages: elastic deformation, plastic deformation, and fracture. The stress-strain curves of metallic Ti samples containing different concentrations of vacancies, self-interstitial impurity atoms, and impurity He atom defects at a tensile strain rate of 2$×$109 s-1 were investigated respectively, and the Young' s modulus was statistically analyzed for different cases. Additionally, the tensile fracture process of metallic Ti containing self-interstitial impurity atoms and impurity He atoms was observed and analyzed respectively.

Full Text

January 2015, Vol. 51, No. 1, pp. 107-113

ACTA METALLURGICA SINICA

A Simulation Study of Mechanical Properties of Metal Ti Sample with Defects

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ABSTRACT

The effect of defects in metal Ti such as vacancies, self-interstitial atoms, and impurity He atoms on the mechanical properties of metal Ti samples was studied using molecular dynamics simulation. First, the stress-strain curves of perfect Ti samples at different strain rates were calculated. The results show that the stretching process can roughly be divided into three stages: elastic deformation, plastic deformation, and fracturing. For comparison, the stress-strain curves of metal Ti samples with vacancies, self-interstitial atoms, and impurity He atoms were researched respectively, with the strain rate set as 2×10^9 s^{-1}. Finally, the corresponding Young' s moduli were calculated. It is found after careful investigation that the mechanical properties of metal Ti are degraded by each of these defects, and the degradation degree increases with increasing defect concentration. However, the stretching process of samples is not essentially affected by these defects (the stress-strain curves of Ti samples with defects still have three stages). In this process, self-interstitial atoms in samples always remain bonded to metal Ti atoms, but impurity He atoms in samples are released due to their extraordinarily low solubility in metal Ti.

KEY WORDS defect, mechanical property, molecular dynamics simulation

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Titanium and its alloys are widely used in engineering applications due to their high melting point, low density (approximately 4.5 g/cm^3), and high specific strength. Therefore, investigating the strain rate dependence of mechanical properties of metal Ti is highly significant. This simulation selected tensile strain rates of 2×10^8, 5×10^8, 1×10^9, 2×10^9, and 5×10^9 s^{-1}.

[Figure 1: see original paper] presents the stress-strain curves of perfect metal Ti samples at different strain rates. It can be observed that under various tensile strain rates, the stress-strain curves of metal Ti can be divided into three distinct stages: (1) In the strain range below 0.05, metal Ti undergoes elastic deformation, where stress increases linearly with strain, following Hooke' s law. During this stage, although Ti atoms deviate from their equilibrium positions, only the lattice dimensions change without breaking of metallic bonds. (2) With continued stretching, in the strain range of approximately 0.05 to 0.12, the stress-strain curves begin to plateau and deviate from linearity, indicating a transition from elastic to plastic deformation and the onset of localized metallic bond rupture. (3) When strain increases to approximately 0.13, stress drops rapidly with increasing strain, and the sample fractures instantaneously. As stretching proceeds, contacting atoms become fewer, and the two ends separate. Linear fitting using the least squares method was applied to the strain range of 0–0.03 in Figure 1, yielding Young' s moduli of approximately 130 GPa for metal Ti samples at all tensile strain rates, which is relatively close to the experimental result of 116 GPa [21].

Table 1 lists the Young' s moduli, tensile strengths, and fracture strains of

perfect metal Ti samples at different tensile strain rates. It can be seen that Young's modulus remains relatively constant at around 130 GPa with increasing strain rate, showing no significant variation. However, both tensile strength and fracture strain increase with increasing strain rate, demonstrating a strain rate strengthening effect.

2.2.1 Mechanical Properties of Metal Ti Samples with Vacancy Defects

To investigate the influence of vacancy defects on the mechanical properties of metal Ti, different numbers of atoms were randomly removed from the interior of perfect Ti samples to create samples with vacancy concentrations of 0.4%, 0.9%, 2.7%, 4.6%, 7.3%, and 9.2%. These samples were then stretched at a strain rate of 2×10^9 s^{-1}, and the resulting stress-strain curves are shown in Figure 2a [Figure 2: see original paper]. Regardless of the vacancy concentration, the shape of the stress-strain curves does not change fundamentally; the stretching process still undergoes three stages: elastic deformation, plastic deformation, and fracture. However, the fracture strain and tensile strength of samples with vacancy defects are lower than those of perfect lattice metal Ti, and both decrease gradually with increasing vacancy concentration, as shown in Table 2 . Linear fitting using the least squares method was applied to the strain range of 0–0.03 in Figure 2a, revealing the variation of Young' s modulus with vacancy concentration, as shown in Figure 2b [Figure 2: see original paper]. The Young' s modulus exhibits a basically linear inverse relationship with vacancy concentration, and the decrease is substantial. The Young' s modulus of metal Ti with a vacancy concentration of 9.2% is 76 GPa, representing a 41.5% decrease from the 130 GPa of the perfect lattice, indicating that vacancy defects severely affect the mechanical properties of metal Ti.

2.2.2 Mechanical Properties of Metal Ti Samples with Self-Interstitial Atoms

To study the effect of self-interstitial atom defects on the mechanical properties of metal Ti, 200, 500, 800, 1000, and 2000 Ti atoms were added at random positions within perfect metal Ti samples to create samples with self-interstitial atom concentrations of 0.3%, 0.8%, 1.3%, 1.6%, and 3.1%. These samples were stretched at a tensile strain rate of 2×10^9 s^{-1}, and the resulting stress-strain curves are presented in Figure 3a [Figure 3: see original paper]. Unlike vacancy defects, while the fracture strain and tensile strength of the simulated system with self-interstitial atom defects are lower than those of perfect lattice Ti, their variation with defect concentration is not obvious, as shown in Table 3 . Linear fitting using the least squares method was applied to the stress-strain curves in the strain range of 0–0.03 in Figure 3a, revealing that Young' s modulus decreases linearly with increasing self-interstitial atom concentration, as shown in Figure 3b [Figure 3: see original paper]. The decrease in Young' s modulus is also substantial; for a metal Ti sample with a self-interstitial atom concentra-

tion of 3.1%, Young' s modulus decreases from 130 GPa for the perfect lattice to 110 GPa. The effect of self-interstitial atoms on Young' s modulus is basically equivalent to that of vacancy defects, indicating that self-interstitial atom defects also significantly degrade the mechanical properties of metal Ti.

Figure 3a also shows that the presence of self-interstitial atoms does not fundamentally alter the stress-strain curves of the simulated samples; the stretching process can still be divided into three stages. Figure 4 [Figure 4: see original paper] shows the morphologies of a metal Ti sample with a self-interstitial atom concentration of 3.1% at different strains, where an orange sphere represents a lattice Ti atom and a green sphere represents a self-interstitial Ti atom. Figure 4a shows the morphology at a strain of 0.05. Although metallic bonds are stretched and deformed, they have not broken. As can also be seen from Figure 3a, the stress-strain relationship remains linear in the strain range of 0–0.05, indicating elastic deformation. Figure 4b shows the sample morphology at a strain of 0.10, where some metallic bonds have broken, indicating the onset of plastic deformation. This stage corresponds to the strain range of 0.05–0.10 in Figure 3a, where the stress-strain curve begins to plateau and deviate from linearity. Figures 4c and 4d show the sample morphology after fracture. As stretching proceeds, contacting atoms become fewer and the two ends separate, corresponding to the stress-strain curve in Figure 3a for strains greater than 0.1, where stress drops sharply with continued strain increase.

2.3 Mechanical Properties of Metal Ti Samples with Impurity He Atoms

To investigate the influence of impurity He atoms on the mechanical properties of metal Ti, 200, 500, 800, 1000, and 2000 He atoms were sequentially added at random positions within perfect metal Ti samples to create samples with He atom impurity concentrations of 0.3%, 0.8%, 1.3%, 1.6%, and 3.1%. These samples were also stretched at a tensile strain rate of 2×10^9 s^{-1}, and the resulting stress-strain curves are shown in Figure 5a [Figure 5: see original paper]. He atom impurities similarly do not fundamentally affect the stress-strain curves; the stretching process can still be divided into three stages, consistent with the results for vacancy and self-interstitial atom defects. Linear fitting using the least squares method was applied to the stress-strain curves in the strain range of 0–0.03 in Figure 5a, revealing the variation trend of Young' s modulus with impurity He atom concentration, as shown in Figure 5b [Figure 5: see original paper]. Similar to vacancy and self-interstitial atom defects, Young' s modulus exhibits a linear inverse relationship with impurity He atom concentration, but the effect of impurity He atoms on Young' s modulus is slightly smaller than that of the former two defect types.

Table 4 lists the Young' s moduli, tensile strengths, and fracture strains of metal Ti samples with different impurity He atom concentrations at various tensile strain rates. The tensile strength and fracture strain both decrease with increasing impurity He atom concentration, and the decrease in tensile strength

is substantial. For example, the tensile strength of perfect metal Ti is 10.68 GPa, while that of a sample with 3.1% impurity He atoms decreases to 6.33 GPa—a reduction of nearly 41%, which is greater than the effect caused by the same concentration of self-interstitial defects. In summary, impurity He atom defects also significantly degrade the tensile mechanical properties of metal Ti samples.

Figure 6 [Figure 6: see original paper] shows the morphologies of a metal Ti sample with an impurity He atom concentration of 3.1% at different strains, where an orange sphere represents a lattice Ti atom and a blue sphere represents an impurity He atom. Figure 6a corresponds to the elastic deformation stage, Figure 6b to the plastic deformation stage, and Figures 6c and 6d to the fracture stage. Comparing the stretching process of metal Ti samples with impurity He atoms (Figure 6) to that of samples with self-interstitial atoms (Figure 4) reveals that during the tensile fracture of metal Ti, self-interstitial atoms remain constrained within the sample due to metallic bonding, whereas impurity He atoms near the fracture surface are released from the sample. This occurs because He atoms, as inert gas atoms, have extremely low solubility in metal materials [22–24] and readily diffuse at interstitial positions [22,25], allowing He atoms near the fracture surface to easily escape. In contrast, self-interstitial atoms form strong metallic bonds with the host Ti atoms, which firmly bind them within the sample and prevent their release.

Conclusions

(1) Calculations of stress-strain curves for perfect lattice metal Ti at different tensile strain rates reveal that strain rate affects the mechanical properties to some extent but does not fundamentally alter the stretching process, which can always be divided into three stages: elastic deformation, plastic deformation, and fracture.

(2) The presence of all three defect types—vacancies, self-interstitial atoms, and impurity He atoms—degrades the mechanical properties of metal Ti, with more severe effects at higher defect concentrations. However, these defects do not fundamentally change the stretching process.

(3) Observation and analysis of the tensile fracture process of metal Ti containing self-interstitial atoms and impurity He atoms show that during tensile fracture, self-interstitial atoms remain constrained within the sample due to metallic bonding, while impurity He atoms near the fracture surface are released because of their extremely low solubility in metal Ti.

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Note: Figure translations are in progress. See original paper for figures.