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Probing influence of void defect on mechanical and deformation behavior of AlCoCrFeNi high-entropy alloy: A molecular dynamics approach

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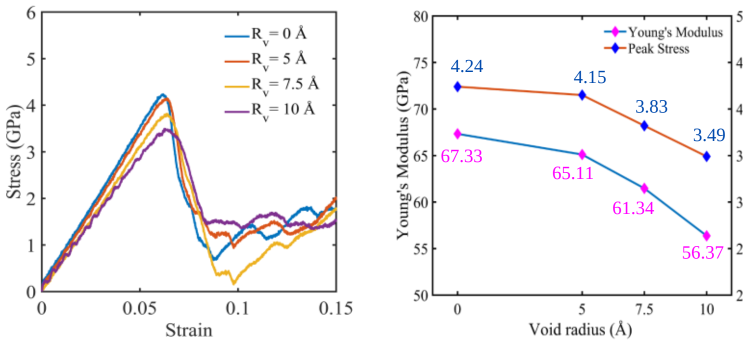
1. INTRODUCTION AND OBJECTIVE

High-entropy alloys (HEAs) are an advanced type of material made up of four or five principal elements in nearly identical atomic percentages [1] or atomic fractions ranging between 5-30% for each alloying component [2]. These materials display exceptional mechanical characteristics [3], making them attractive for several applications, such as aerospace, automotive, energy, and biomedical engineering [4]. AlCoCrFeNi HEAs have been widely investigated both experimentally and computationally among the numerous reported HEAs by researchers. For instance, Wang et al. [5] studied the evolution of the microstructure of $Al_xCoCrFeNi$ (x=0-1.8 in molar ratio) HEAs under varying temperatures and Al concentrations. The mechanical properties of these HEAs are affected not only by the types and concentrations of alloying elements but also by the defects that arise during the fabrication process. Needleman and Tvergaard [6] demonstrated that void coalescence is the primary failure mechanism in single-crystal copper. Gao et al. [7] performed MD simulations to explore the mechanical properties and deformation behavior of FeNiCrCoCu HEA under tensile loading while taking into account cylindrical voids with different sizes and numbers. Doan et al. [8] reported the impact of void and inclusion size on the mechanical and deformation behavior of $AlCoCuFeNi_2$ HEA under uniaxial tension. Their results showed that as the void size increased, the mechanical characteristics decreased. However, the influence of voids on the mechanical properties and deformation behavior of AlCoCrFeNi HEA remains unclear. Therefore, this study aims to investigate the influence of void defect on the stress-strain response and deformation behavior of AlCoCrFeNi HEA under tensile loading through MD simulation.

2. RESULTS & HIGHLIGHTS OF IMPOINTANT POINTS

Fig. 2(a) displays the influence of different void sizes on the stress-strain responses of AlCoCrFeNi HEA under uniaxial tension. The stress-strain response of AlCoCrFeNi HEA that has no void ($R_v = 0$ Å) is compared to the stress-strain responses of AlCoCrFeNi HEA with void radii of $R_v = 5$, 7.5, and 10 Å. All stress-strain responses display a linear increment in the elastic regime, reaching a peak stress value. The peak stress of AlCoCrFeNi HEA with no void is 4.24 GPa, which is higher than the peak stress (4.15 GPa) of AlCoCrFeNi HEA with a void radius of $R_v = 5$ Å. As the void size increases from $R_v = 5$ Å to $R_v = 10$ Å, the peak stress decreases from 4.15 GPa to 3.49 GPa. The peak stress of AlCoCrFeNi HEA with a void radius of $R_v = 10$ Å is 17.68% and 15.90% lower than the peak stress of AlCoCrFeNi HEA with no void and a void radius of $R_v = 5$ Å, respectively. This indicates that void defects, especially with increased sizes, degrade the tensile strength of HEAs, which is consistent with previous findings [7,8]. After reaching the peak stress, the stress-strain responses decrease sharply, indicating the yielding of the HEA followed by plastic deformation. As the strain increases, the plastic deformation progresses with continuous stress fluctuations. Fig. 1(b) shows the effect of void sizes on Young's modulus, revealing that Young's modulus decreases by 13.42%, from 65.11 GPa to 56.37 GPa, as the void radius increases from 5 Å to 10 Å. The Young's modulus of AlCoCrFeNi HEA with no void is 67.33 GPa, which is 19.44% higher than Young's modulus of AlCoCrFeNi HEA with a void radius of 10 Å. Moreover, Fig. 1(b) demonstrates the decrease in peak stress and Young's modulus of AlCoCrFeNi HEA with increasing void sizes.



(a) (b)

Fig. 2: Mechanical behavior of AlCoCrFeNi HEA with and without internal void defects at the centre; (a) Stress-strain responses of AlCoCrFeNi HEA without voids ($R_v = 0$ Å) and with voids of different sizes ($R_v = 5$, 7.5, and 10 Å); (b) Corresponding Young's modulus and peak stress of AlCoCrFeNi HEA.

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