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گواهی ثبت مقاله در سیویلیکا
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عنوان مقاله:

Molecular dynamics simulation of temperature effects on the mechanical properties of Carbon polycrystalline

محل انتشار:

The Progress in Physics of Applied Materials, دوره 4, شماره 1 (سال: 1403)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

The mechanical properties of carbon polycrystalline materials are crucial because they determine how the material responds to external forces, such as stress and strain, and environmental conditions. By investigating the mechanical properties of carbon polycrystalline materials, researchers can develop insights into their strength, ductility, hardness, and other characteristics, which are vital for their practical applications in industries such as manufacturing, construction, and materials science. Molecular dynamics techniques enable the examination of various polycrystalline configurations and the assessment of their effectiveness. The present study investigates the effects of temperature on the mechanical properties of Carbon polycrystalline. The results show that the ultimate strength and Young's modulus of the simulated polycrystal are ۶۴.۵۵۳ Gpa and ۳۵۵.۲۸۴ GPa, respectively. Also, the results showed that with increasing temperature to ۳۲۰ K, Young's modulus and ultimate strength of carbon polycrystalline increase to ۳۶۳.۱۸۵ and ۶۹.۴۱۷ GPa, respectively. With a further increasing the temperature to ۳۵۰ k, these parameters decrease to ۳۴۹.۹۰۹ and ۶۳.۰۴۷ GPa. The observed increase in these parameters at lower temperatures may be attributed to the increased atomic mobility of the samples resulting from the initial temperature enlargement. The simulation results .are expected to help further understand the influence of temperature on the mechanical properties of carbon polycrystalline materials

کلمات کلیدی:

Molecular dynamics simulation, Temperature, Mechanical properties, Polycrystalline

لینک ثابت مقاله در پایگاه سیویلیکا:

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