عنوان مقاله:

Molecular Dynamics Simulation of Melting Point of Molybdenum Dioxide

محل انتشار:

هفتمین کنفرانس بین المللی مهندسی مواد و متالورژی و دوازدهمین همایش ملی مشترک انجمن مهندسی متالورژی و مواد ایران و انجمن ریخته گری ایران (سال: 1397)

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خلاصه مقاله:

Highly ordered mesoporous crystalline MoO2 materials with bicontinuous Ia3d mesostructurewere synthesized by using phosphomolybdic acid as precursor and mesoporous silica KIT-6as hard template in 10% H2 atmosphere via nano casting strategy. The prepared mesoporousMoO2 material shows typical metallic conductivity with low resistivity (~0.01Ω cm at 300K), which makes it different from all previously reported mesoporous metal oxides materials.We have calculated here the melting point of molybdenum dioxide by simulating moleculardynamics and its ReaxFF potential.

کلمات کلیدی:

Molybdenum Dioxide, Molecular Dynamics, Melting Point, Heat Capacity