عنوان مقاله:

The effect of temperature rise rate on graphene sublimation

محل انتشار:

پنجمین کنفرانس بین المللی فیزیک، ریاضی و توسعه علوم پایه (سال: 1400)

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نویسندگان:

Mohsen Yarifard – Department of Physics, Qazvin Branch, Islamic Azad University, Qazvin, Iran

.Jamal Davoodi – Department of Physics, Zanjan University, Zanjan, Iran

خلاصه مقاله:

In this paper, using molecular dynamics simulation, graphene phase transition with respect to enthalpy and mean square displacement of particle changes in terms of temperature is investigated. Graphene is converted to gaseous carbon chains due to temperature rises. Bond length between the carbon atoms in these carbon chains is shorter than the bond length in graphene. The results demonstrate that the sublimation temperature and latent heat of sublimation increase as a function of temperature rise rate. Therefore, to achieve the laboratory value of these quantities using simulation, the temperature rise rate .should be as low as possible

کلمات کلیدی:

Graphene, Molecular dynamics simulation, Sublimation