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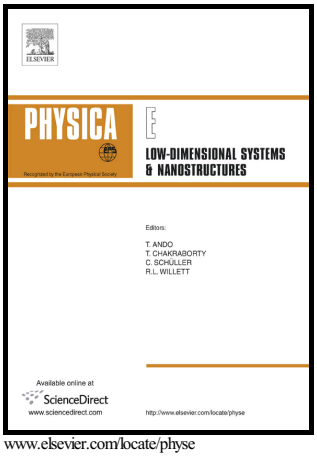

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Abstract:

A molecular structural mechanics model for the numerical simulation of phonon dispersion relations of graphene is developed by relating the C-C bond molecular potential energy to the strain energy of the equivalent beam-truss space frame. With the stiffness matrix known and further based on the periodic structure characteristics, the Bloch theorem is introduced to develop the dispersion relation of graphene sheet. Being different from the existing structural mechanics model, interactions between the fourth-nearest neighbor atoms are further simulated with beam elements to compensate the reduced stretching stiffness, where as a result not only the dispersion relations in the low frequency field are accurately achieved, but results in the high frequency field are also reasonably obtained. This work is expected to provide new opportunities for the dynamic properties analysis of graphene and future application in the engineering sector.

Keywords: graphene sheet; energy equivalence; beam-truss space frame; phonon dispersion relation; low-dimensional nanostructure.

1. Introduction