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Phonon instability and charge density wave in U_2Ti

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Phonon instability and charge density wave in U_2Ti.

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Abstract

Phonon dispersion, structural distortion and the elastic properties of U_2Ti are studied using ab-initio techniques. Our calculations revealed an instability in the hexagonal structure of U_2Ti which is not observed in the earlier studies on this system. This instability is demonstrated through the imaginary phonon frequencies found around the A-point in the Brillouin zone. This instability leads to a Peierl's type of dimerization of U atoms along Z direction which will result in the formation of charge density wave (CDW) in the system. The dimerization leads to a new ground state structure in the system whose unit cell evolve by the doubling of the original cell along the Z direction. Our calculations further showed that the CDW exist in the system up to a pressure of 4 GPa.

Key words: Actinide alloys and compounds, U_2Ti, Electronic band structure, Phonon

1. Introduction

Studies on the uranium compounds and alloys have continued to attract attention for many years due to their application as nuclear fuel materials. These materials have also been of interest to solid state community as the 5f electrons in these systems are at the verge of delocalisation. These 5f electrons give rise to many interesting phenomena like Mott insulating behaviour in UO_2, heavy

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