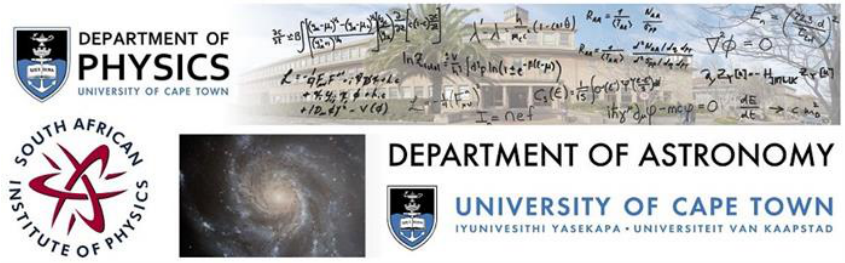

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First Principle Investigation of Structural, Thermodynamic, Electronic and Elastic Properties of Ru-Cr-Z Ternary Alloys

Tuesday, 5 July 2016 14:20 (20 minutes)

Abstract content
   (Max 300 words)
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We report the first principle structural, elastic, thermodynamic, and electronic properties of Cr-Ru-X ternary alloys (where X = V, Mo, Fe, Pd and Mn) obtained from the density functional theory. The heats of formation, bulk modulus, density of states, elastic constants and the band structure energy are calculated and systematically compared to available theoretical and experimental data. The calculated heats of formation predicted an improved stability when the systems are doped with six atoms of Mo, Mn and Fe atoms. Band structures of Ru-rich and Cr-rich alloys indicate an overlap between the valence and the conduction band hence our systems are metallic with a zero band gap. Furthermore the elastic constants of the studied systems are predicted as mechanically stable under the Born criterion of cubic structures. The ratio of bulk to shear modulus was used to determine the ductility/brittleness of the material.

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