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Ab initio thermodynamic and elastic properties of Pt-Cr binary alloys

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<p>Planewave pseudopotential calculations were conducted to predict the phase stability of Pt-Cr binary alloys. The heats of formation are determined for five different phases, L12, A15, DOC, DO'C and tP16 of Pt3Cr and PtCr3. We observed that the cubic L12 Pt3Cr is the most stable structure in agreement with the experiments. The results for PtCr3 indicate the negative heat of formation for the A15 phase whereas all the remaining studied phases have positive heats of formation. In addition the phase stability study was performed on two phases, B2 and L10 of the PtCr alloy. L10 phase was found to be more stable compared with the PtCr B2 phase. Elastic constants and moduli were investigated to determine the strength of the Pt-Cr systems. The strength of PtCr L10 is greater than that of B2 phase. The ratio of shear to bulk modulus (G/B) has been used to predict the ductility or the brittleness of the material.

Level (Hons, MSc,
   PhD, other)?

PhD

Consider for a student
   award (Yes / No)?

No

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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