

Theoretical study of lattice constants, thermodynamic stability and elastic properties of Pt-Ir-X solid solution phases

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Abstract

Lattice constants, thermodynamic stability and elastic properties of Pt-Ir-X (X=Ag, Au, Cu and Mo) systems were studied by ab initio calculations and CALPHAD modeling. The lattice constants and energy of formation of the Pt-X and Ir-X systems were calculated by DFT and compared with the XRD and CALPHAD results. The diffusion barrier of the constituent binary systems was simulated by DFT and the driving force of phase separation was derived from CALPHAD. Young's moduli of Pt-Ir were calculated by DFT, which shows a good agreement with the experimental data. The results demonstrate that ab initio calculations and CALPHAD modeling can be applied together to perform a comprehensive study on microstructural, thermodynamic, kinetic and elastic properties of materials.