

## Pseudopotential study of lattice parameter and heat of formation for substitutional alloys

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**Abstract.** Ashcroft's empty core pseudopotential is applied to the substitutional alloy (K-CS) to calculate the heat of formation and lattice parameter over the entire concentration range. At any concentration the defect crystal is considered to be equivalent to a perfect crystal with a modified lattice parameter and the potential parameter for the defect crystal is calculated by using some suitable interpolation formula. The calculated results agree well with the available experimental results.

**Keywords.** Ashcroft pseudopotential; substitutional alloy; heat of formation; lattice parameter; Vegard's law.

### 1. Introduction

The study of pure metals on the basis of pseudopotential theory has made spectacular progress during the past few years. The formalism is so powerful that Cohen (1979) describes it as a 'panacea' in solid state physics. Static properties of alkali metals can reasonably be well reproduced by Ashcroft's model potential. Recently Sen and Sarkar (1980) have made a unified study of alkali metals on the basis of Ashcroft's (1966) model potential and obtained fairly good agreement for most of the static properties.

The above facts led us to investigate how much effective is the pseudopotential method in describing the properties of substitutional alloys. Several attempts (Tanigawa and Doyama 1973; Singh and Young 1972; Zhernov and Solt 1977) have already been made to calculate the heat of formation of metallic alloys. Tanigawa and Doyama (1973) calculated the heat of formation of (K-Rb) and (Rb-CS) alloys using Ashcroft's pseudopotential. They assumed Vegard's (1921) law for the lattice parameter and determined the lone parameter  $r_c$  for the alloys from the equilibrium condition. The values of  $r_c$  determined in this way is found to vary linearly with concentration and the heat of formation calculated with these values of  $r_c$  shows discrepancy upto 300%. Zhernov and Solt attempted a better calculation using local Heine-Abarenkov potential and considering local distortion and change in vibrational energy. They used Harrison's (1966) prescription that the average form factor of an alloy at a particular concentration is given by the weighted average of the form factors of the host and impurity crystals. Though the theoretical basis of their calculation seems to be sound the calculated values of heat of formation for (K-CS) shows a discrepancy no less than 600%.