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DISTRIBUTION OF THE LATTICE ENERGY IN CUBIC CRYSTALS AND ITS VARIATION WITH COMPRESSION OR EXPANSION*

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Abstract—The total lattice energy of face-centred and body-centred cubic crystals has been calculated on the assumption of a pair-wise interaction potential, for a variety of such potentials. These were either of Morse or Mie (Lennard–Jones) type, with the parameters adjusted to minimize the total lattice energy for an ideal unstrained crystal at 0°K. The same potentials were used to compute the variation in lattice energy when the lattice is allowed to expand or contract by up to 2·5 per cent. The relative contributions of different interactions to the total energy are given. For face-centred cubic crystals, most potentials predict a major contribution from nearest-neighbour interactions, although the contributions of second and higher neighbours are still significant. For body-centred cubic crystals, the dominant contribution usually comes from the second neighbour interactions. Some typical variations in these contributions with changes in lattice parameter are given.

1. INTRODUCTION

IN THIS paper, we assume that the total lattice energy (cohesive energy) of a crystal can be calculated as the sum of pair-wise interactions between all atoms. Various forms are considered for the interaction potential function, in all of which the parameters have been adjusted to minimize the lattice energy for an ideal unstrained crystal at 0°K. The lattice energy is then calculated for body-centred and face-centred cubic crystals, first for a lattice parameter corresponding to this minimum energy and then also for parameters deviating from this value by a few per cent. Such changes in lattice energy may be expected if the crystal is at higher temperatures or under hydrostatic pressure. Clearly any vibrational contribution to the lattice energy is not taken into account in this calculation. Corresponding calculations of surface energy are discussed in the following paper.[1]

The calculation of energies by summing pair-wise interactions has been used previously by many authors,[2,3] despite the recognition that many-body interactions may make a significant contribution to the total energy.[4] The attractions of the method are that it is mathematically tractable and that it does appear to provide a good approximation in many cases. The pair-wise potential itself can be chosen either as a "real" potential derived from quantum-mechanical calculations or as a "fictitious" potential[2] of simple mathematical form and containing one or more adjustable parameters. The second approach is more in keeping with the philosophy of the method and may be expected to give a better approximation when the parameters are chosen to fit some specific experimental data.

As discussed in detail in Section 2, we have restricted our calculations to Morse and Mie

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