ABSTRACT

Interatomic potentials employing non-central forces have been developed for fcc metals and used to determine the minimum energy configurations of interstitial defects in these materials. In the bcc metals, central potentials were developed and used to calculate vacancy migration energies and divacancy binding energies. Phonon dispersion curves were also calculated using these models.
1 INTRODUCTION

In an attempt to simulate defects in metals, extensive lattice-model calculations have been carried out on the basis of two-body interatomic potentials. Behind all such calculations is the principle that changes in the lattice energy can be written as a function of the positions of the atoms comprising the metal. Various schemes for determining the parameters of this energy function have been based on empirically fitting known physical properties of the metal, on theoretical considerations, or on combinations of the two (semiempirical methods).

When any empirical fitting is used to help determine the parameters of the energy function, there is no uniqueness to the result: in most cases, any number of quite different models can yield satisfactory agreement. In addition, the physical properties to which the fit is made apply primarily to the perfect lattice, although some defect parameters have been used. Thus the energy function is matched to several known points of configuration space, and then investigated in an entirely different region: the whole process may be thought of as very complicated curve fitting to one part of configuration space and extrapolation to another region. There is no a priori way of knowing whether this extrapolation is reasonable, i.e., whether the forces which describe the crystal at the fitted points are adequate to describe the defect state.

In the present work (both this paper and the paper Rare Gases in Metals), a combination or semiempirical approach has been used to develop interatomic potentials. Calculations have been carried out over a wide range of materials and defect configurations in an effort to obtain as complete an understanding of the applicability of those potentials as possible. Since this work essentially involves an extension of earlier calculations (e.g., Johnson$^1$, Wilson and Johnson$^2$, and Wilson and Bisson$^3$), much of the background material and rationale for those studies is not repeated here. Accordingly, this paper is divided into two basic sections; the development of the interatomic potentials, and the results of calculations with those potentials. The calculational methods used to find the appropriate minima or saddle points in the energy function corresponding to defect configurations is also outlined.

2 INTERATOMIC POTENTIALS

Interatomic potentials for both fcc metals (Ni, Cu, Pd, Ag, and Au) and bcc metals (V, Fe, Mo, Ta, and W) are developed in this section. Although the details are different for the two metal structures, the outline for the development of the potentials is the same: The potentials are short ranged (first nearest neighbor for fcc, first and second nearest neighbor for