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Pseudopotential Calculations of Lattice Distortions around Impurities in Simple Metals

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Second-order pseudopotential calculations are known to reproduce fairly well the structure and phonon spectra of many simple metals (without *d*-states close to the Fermi level) [Heine, V. & Weaire, D. (1971). *Solid State Physics*, **24**, 249–463]. The underlying assumption of linear screening should also be reasonable for impurities with valences and core radii close to those of the host. Its validity can be checked *a posteriori* and by comparing calculated properties with measurements on dilute alloys (lattice expansion, heat of solution, electron scattering lifetime) [Benedek, R. & Baratoff, A. (1973). *Solid State Commun.* **13**, 385–388] and, especially, coherent elastic neutron scattering [Schumacher, H., Schmatz, W. & Seitz, E. (1973). *Phys. Stat. Sol.* (*a*), **20**, 109–117]. The resulting description in terms of pairwise screened host–host and impurity–host interactions, in conjunction with the lattice-statics approximation [Matsubara, T. J. (1952). *J. Phys. Soc. Japan*, **7**, 270], enables one to carry out a self-consistent calculation of the static structure factor $S(q)$ to first order in the displacements. The calculations to be reported on alkalis in alkalis and on impurities in aluminum are based on Shaw's optimized model potential and on a screening approximation satisfying the compressibility sum rule [Shaw, R. W. (1968). *Phys. Rev.* **174**, 769–781; (1969). *J. Phys. C: Solid State Phys.* **2**, 2335–2449; (1970). *J. Phys. C: Solid State Phys.* **3**, 1140–1158; Vashishta, P. & Singwi, K. S. (1972). *Phys. Rev.* B**6**, 875–887.] Special care has been taken to ensure proper convergence, a problem neglected in previous similar calculations. Calculated structure factors exhibit features associated with appreciable interactions beyond nearest neighbours of the defect and/or with incipient structural instabilities of the host lattice.

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Lattice Distortions by Copper Atoms in an Aluminum Lattice

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With the method of elastic diffuse scattering of neutrons the strain field produced by copper atoms dissolved in aluminum was investigated. Measurements were performed at 800 K and at room temperature on a single crystal containing 0·8 at.% of copper. A time-of-flight technique was applied to discriminate between elastically and inelastically scattered neutrons. The general features of the scattering pattern recorded in the high-temperature run are found to be well explained by a theoretical approach based on the assumption of isotropic forces acting on nearest neighbours only. Possible refinements of the model are discussed. At room temperature the pattern shows the characteristic features resulting from the formation of Guinier–Preston zones.