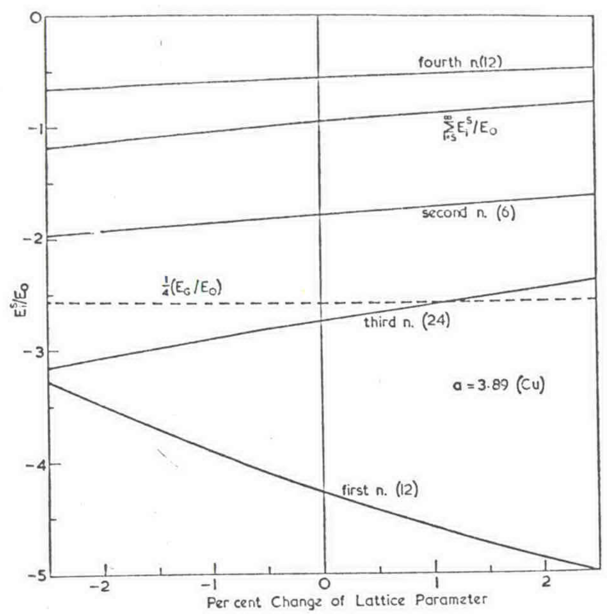

FIG. 5a

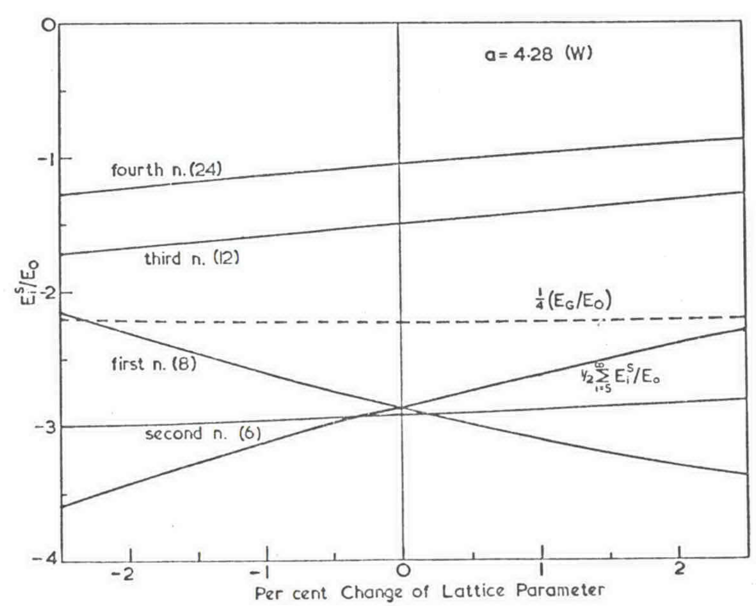

FIG. 5b

FIG. 5. Variations with lattice parameter of various contributions to E_G in (a) a face-centred cubic crystal for a Morse potential of $a = 3{\cdot}89$ and (b) a body-centred cubic crystal for a Morse potential of $a = 4{\cdot}28$; according to (3) these values are appropriate to Cu and W. The number of atoms in each shell of neighbours is given in brackets.

only, particularly for body-centred cubic crystals. One direct example of this has been pointed out by DRECHSLER and LIEPACK[13] in connection with the growth of a (110) face in a body-centred cubic crystal. Here, a single adatom on top of such a face could locate itself on a site with three nearest-neighbours but instead, since growth occurs on such faces, must be located on a site with two nearest and two second-nearest neighbours. This is consistent with detailed calculations with pairwise potentials which show that the latter site has a lower energy.

An interesting demonstration of the effects of distant neighbours has been produced by constructing ball-and-spring models of body-centred and face-centred cubic crystals.[14] Conventional models of this type use springs only between nearest neighbours and since these are made identical they are all in equilibrium for an unstrained crystal. However, the new models use springs between atoms up to third-neighbour separation with spring constants adjusted to fit particular interaction potentials. In these, of course, the nearest-neighbour springs are always in compression and the model gives notably different results from the conventional one when used to study the stability of structures, their elastic properties or the positions of surface atoms relative to their ideal lattice positions.

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