Mini-report on CuPd bcc to fcc transformation

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1 CuPd bcc -> fcc transition

The bcc transforms to fcc through the body centered tetragonal (bct) shape as shown in Figure 1.

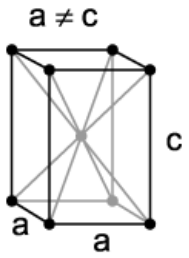

Figure 1: Body Centered Tetragonal Structure

As dimension 'c/a' becomes equal to 1, the bct structure becomes bcc (i.e. 'c'='a'). Similarly, when 'c' becomes equal to the square root of 2, the structure becomes fcc. This is demonstrated graphically in Figure 2.

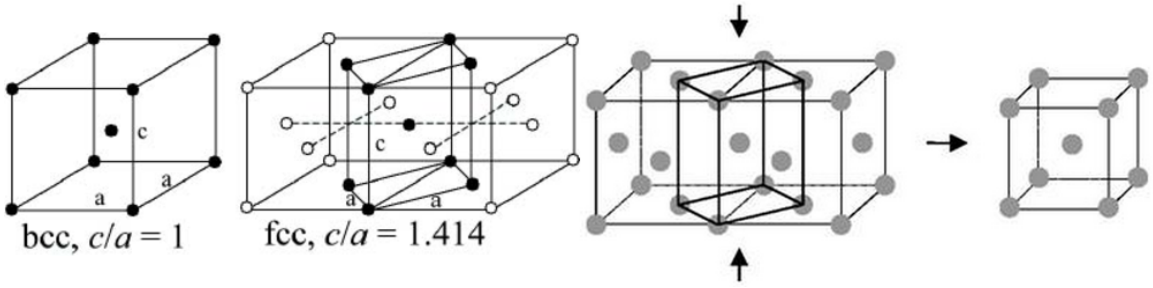

Figure 2: fcc transformation to bcc by shrinking 'c/a' of bct structure

2 Energies of the diffusion pathway

Figure 3 shows a 3-dimensional image of the minimum energy pathway. There is approximately 50meV difference between the two structures. The pathways does not follow a simple path of constant 'a' or 'c'.

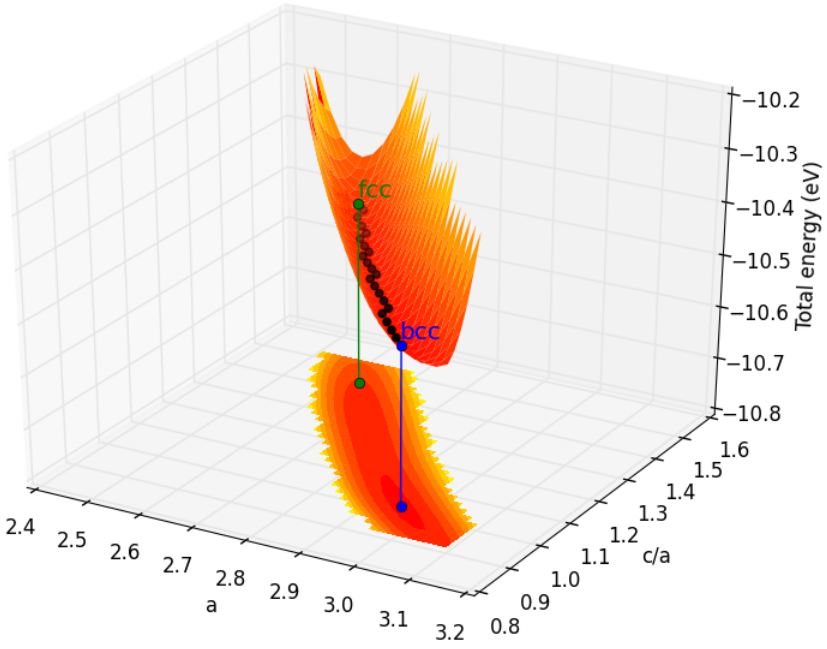

Figure 3: 3D minimum energy well for with changes in the 'a' and 'c/a' properties of the bct structure

Note: lines of constant 'c/a' are representative of equations of state i.e. only volume changes, while the relative magnitudes of the vectors are constant.

The minimum energy pathway is shown via 'c/a' in Figure 4. Interestingly, there is no appreciable barrier to speak of.

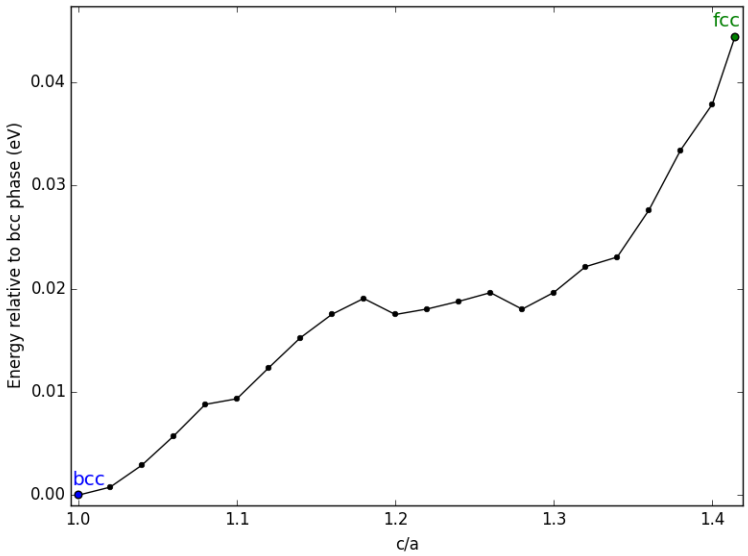

Figure 4: Minimum energy pathway for bcc transformation to fcc