Microsymposium

Polytypism in layered AB_2 solids

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Simple solids such as TaS_2, $NbSe_2$, and CdI_2 show surprisingly complex polytypic behaviour where a number of crystalline structures can form whose unit cells differ only along their c-axis [1, 2]. This phenomena arises due to the differences in stacking sequences of the AB_2 layers along the c-axis. Although models have been developed to explain the complex phase behaviour, no model thus far has been able to account for all polytypes formed in practice [3, 4].

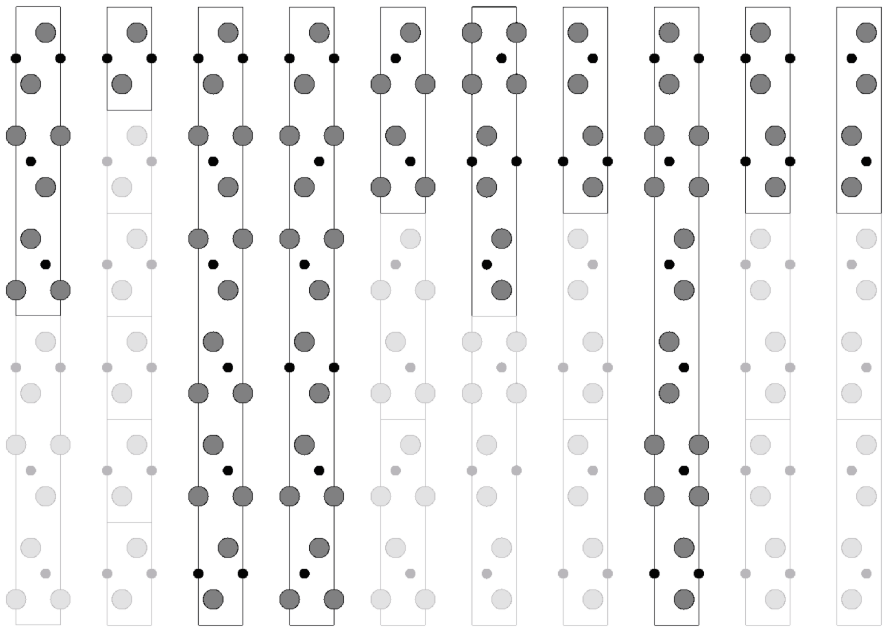

Figure 1. Projection of AB_2 layers onto the (**a,c**)-plane for the ten ground states produced by our model. A cations are shown as small black spheres and B anions are represented by large grey spheres.

In this study we look at a new way of describing the structure of layered AB_2 compounds. Focusing on the layered dichalcogenides, we translate their structural degrees of freedom to a 1D model of coupled Ising chains to explain the polytypic behaviour. Our analysis suggests a family of ten 'simplest' ground states (Figure 1), seven of which have previously been reported. Using Monte Carlo simulations, we find that other phases identified in the literature but not expected by our model, are either describable as disordered states intermediate to our limiting phases, or mischaracterised. We proceed to show that the coupled 1D Ising chains encapsulate the behaviour of solid solutions of layered AB_2 systems, with a long term aim to link the properties of these materials to the interaction parameters relevant to the model. This phase control is an important result as it could lead to targeted design for specific properties, as structure is known to have a profound influence on materials' properties.

[1] Katzke, H., Tolédano, P. & Depmeier, W. (2004). *Phys. Rev. B* **69**, 134111.

[2] Wahab, M.A. & Kant, R. (1986). *Cryst. Res. Technol.* **21**, 243-251.

[3] Trigunayat, G. C. (1989) *Phase Transit.* **16**, 509.

[4] Ramasesha, S. & Rao, C. N. R. (1977) *Phil. Mag.* **36**, 827.

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