Structural and theoretical studies of [(MX)$_{1+y}$]$_m$[TX$_2$]$_n$ thin film ferecrystals

Inorganic chemists generally can only form extended solids in thermodynamically stable phases. However, it is possible to trap kinetically stable phases in thin films of misfit layered compounds with the chemical formula [(MX)$_{1+y}$]$_m$[TX$_2$]$_n$ (X= S, Se; M= Sn, Pb, Sb, Bi, and rare earth metals and T=Ti, V, Cr, Nb, Ta, Mo, V) by not introducing sufficient energy for overcoming the large activation energy required to form the thermodynamically stable product. Misfit layered materials exhibit a broad range of physical properties and form a structure where the TX$_2$ layer is a single (001)-oriented molecular layer of the transition metal dichalcoginate and the MX layer contains two distorted atomic planes of the rock-salt structure with 001 orientation. The m and n values represent the number of layers in the unit cell of each structure. The materials are referred to as misfit layers because the rock-salt layers are incommensurate with the close packed X planes of the TX$_2$ layers and the misfit parameter, y, is the difference between the density of metal cations in their respective. However, these films are different from traditional misfit layer compounds in that the material is crystalline within the planes, but from plane to plane there is a misorientation between the layers which limits the long range order. We termed these materials ferecrystals, which means “almost crystals”. Here we will present the structural and theoretical work of several of our most interesting ferecrystal materials.