Advanced high-resolution TEM of layered crystals and incommensurate misfit layer compounds and their interfaces

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Materials research for advanced nano-scale and thin film materials, layered structures and interfaces has established itself as a fascinating and attractive research field because of its fundamental importance in understanding the chemical and physical properties of these materials and in evaluating their potential for technological applications. Advanced high-resolution transmission electron microscopy (HRTEM) including the new developments of aberration-corrected HRTEM plays a crucial role in characterizing layered structures and interfaces on the atomic scale which is important for establishing structure-property relationships.

The presentation will summarize electron microscopy investigations of interface and surface phenomena of transition metal dichalcogenide crystals, with a focus on self-assembled surface nanostructures and metal intercalation for layered chalcogenide crystals [1-4] and on the effects of interface incommensurability in epitaxial layers [5] and in misfit layered compounds [6,7].

As an example, Fig. 1 shows the projected crystal structure of the incommensurate misfit layered compound $(PbS)_{1.14}NbS_2$ and the corresponding diffraction pattern revealing the incommensurability by an irrational spacing of lines of reflections arising from the two subsystems PbS and NbS_2. Fig. 2 demonstrates that direct imaging of the atomic structure becomes possible with aberration-corrected HRTEM whereas conventional HRTEM fails to produce directly interpretable image contrast. One of the reasons for this behaviour is the strong suppression of image delocalization due to aberration-correction which is illustrated by the image intensity simulations in Fig. 3 [7]. By applying aberration-corrected HRTEM, the positions of atomic columns can be determined with high precision allowing the atomic structure to be determined not only in defect-free areas of the crystal but also in the presence of local inhomogeneities and crystal defects [6].

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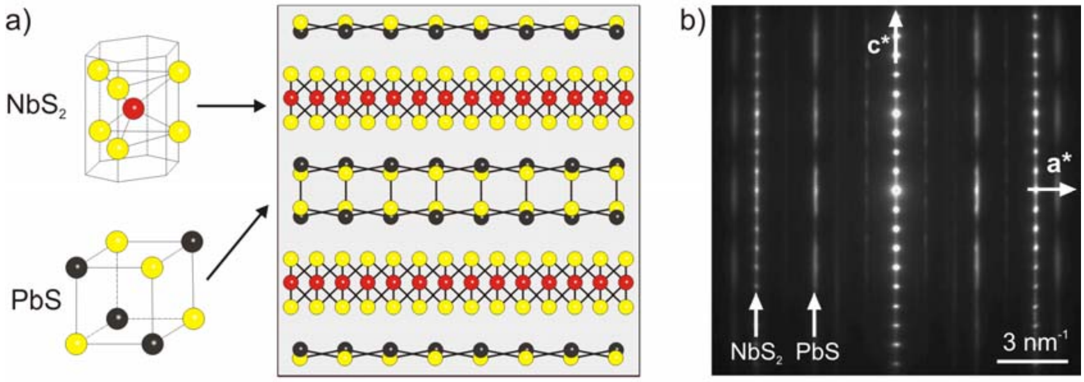

Figure 1. Crystal structure of the incommensurate misfit layered compound $(PbS)_{1.14}NbS_2$ projected along the commensurate interface direction and corresponding electron diffraction pattern.

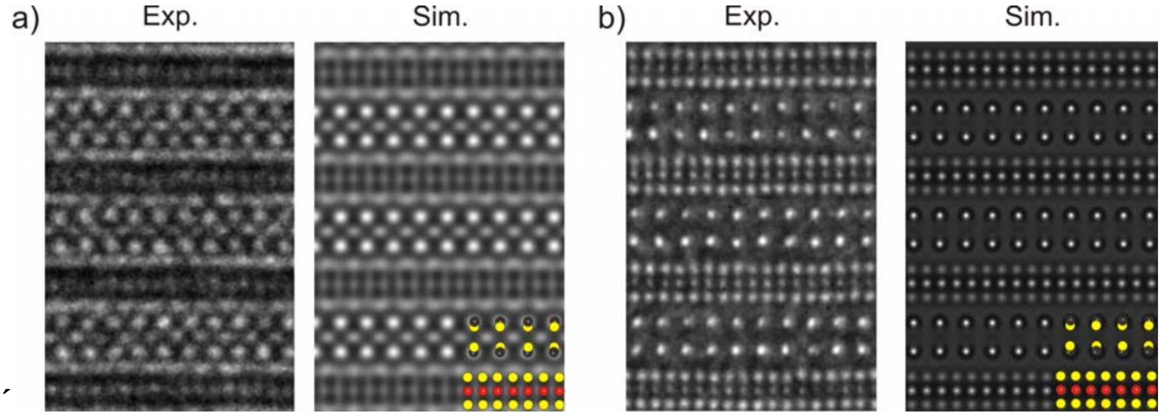

Figure 2. Comparison of experimental and simulated HRTEM images for a $(PbS)_{1.14}NbS_2$ crystal imaged along the commensurate interface direction. a) Conventional HRTEM and b) aberration-corrected HRTEM imaging under NCSI conditions [7].

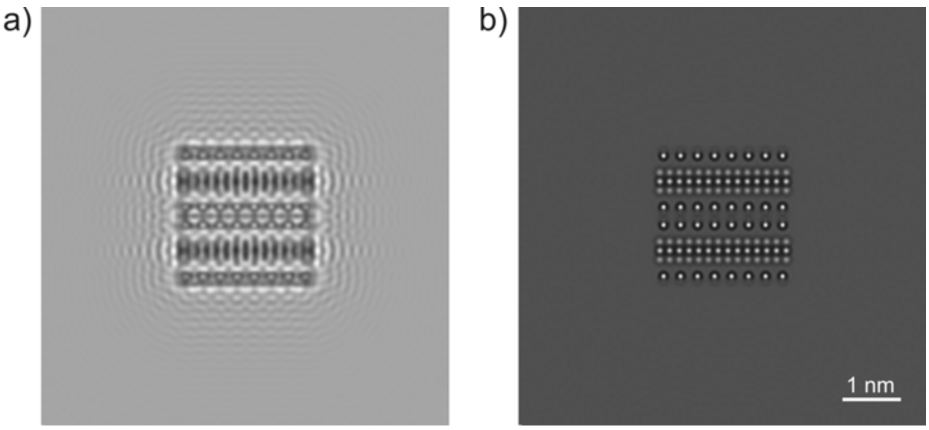

Figure 3. Illustration of the effect of image delocalization for a single unit cell of $(PbS)_{1.14}NbS_2$ (Fig. 1a) embedded in vacuum. a) Multislice simulation of a conventional HRTEM image. b) Corresponding multislice simulation for NCSI-conditions in aberration-corrected HRTEM [7].