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Nanohardness change of silicon and sapphire substrates by TiC/VC multilayers. Peter Paufler^a, Andre Belger^b, Marianne Reibold^c, ^aTU Dresden, FR Physik, Inst.f. Strukturphysik. ^bOn leave of^a. ^cTriebenberg Laboratory, TU Dresden.
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The nanohardness of multilayer specimens TiC/VC @Si und TiC/VC @Sapphire prepared by Pulsed-Laser-Deposition (Nd-YAG laser 355nm) has been investigated to check the existence of a supermodule effect similar to that reported by [1] with TiN/VN. The multilayer period thickness λ varied between 1.34nm and 24.8nm (total layer thickness ~200nm). Nanohardness H was improved, regardless of t , by covering Si as well as sapphire with the TiC/VC multilayer. The maximum value of H obtained was 38 GPa for TiC/VC @Sapphire. Individual hardness of the multilayer and the substrate could be separated by extrapolation the dependence on λ . The results are $H(\text{ML on Si}) = 32.9$ GPa, $H(\text{ML on sapphire}) = 41.5$ GPa, $H(\text{Si}) = 13$ GPa, $H(\text{sapphire}) = 30$ GPa. The multilayer on Si substrate carries 45% of the total load whereas the same layer on sapphire carries only 5%. The rest is due to the substrate. A maximum of H was observed for a multilayer thickness of $\lambda = 10$ nm for both substrates, i.e., a superlattice hardening effect has been detected. Young's modulus E_r , however, did not exhibit a pronounced maximum as function of λ . The beginning of plastic deformation during indentation manifested itself by pop-ins along the force-penetration curve. The critical load was higher for the pop-in registered with the multilayer on sapphire than for sapphire without layer. High-resolution transmission electron microscopy showed that the multilayers are nanostructured. Hardness obeys, as a function of λ , a Hall-Petch relation $H = 35.3 + 6.9 \lambda^{-0.5}$ (H in GPa und λ in nm). Obstacles for dislocation movement are boundaries between nanocrystalline particles, the size of which depends on the annealing history.

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Transmission electron microscopy on stable and metastable Ge/Sb/Te phases. Tobias Rosenthal, Matthias Schneider, Oliver Oeckler *Department of Chemistry, LMU Munich, Germany.*
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Metastable crystalline phases are crucial in the read-erase cycle of GST (Ge/Sb/Te) phase-change materials (PCMs). Whereas they seemingly exhibit strongly disordered rocksalt-type structures, [1] the corresponding stable phases [2] are characterized by layer-like cation defect ordering. This involves the relaxation of Te atoms in a fashion that means the formation of van der Waals gaps rather than that of defect layers in an undistorted matrix. The thermodynamically stable layered phases can be gradually approached by annealing processes, especially if the rocksalt-type phase is stable at high temperatures and metastable states are accessible by quenching. The partially ordered phases thus obtained are

interesting model systems for PCMs but in addition exhibit remarkable thermoelectric properties.

The real structure of such metastable compounds $(\text{Sb}_2\text{Te}_3)_n(\text{GeTe})_m$ ($4 < n < 20$) has been investigated by electron diffraction and microscopy. HRTEM and STEM-HAADF clearly reveal both the extension, relative orientation and frequency of defect layers as well as the local relaxation of atoms near them. Whereas the Te atom positions of the rocksalt-type phase are approximately retained near the limits of defect layers and throughout defect layers that extend over just few unit cells of the basic structure, Te-Te contacts form whenever the cation defect layers extend over larger areas. The frequency of defect layers is determined by the stoichiometry. If the GeTe content is low, the structure contains numerous defect layers which are perpendicular to all $\langle 111 \rangle$ directions of the cubic basic structure, however, their 2D extension is very limited. This results in a parquet-like domain structure. If there are less defect layers, they tend to arrange in a parallel fashion that is similar to the block structures of the thermodynamically stable phases but involves blocks or irregularly varying thickness. At very high GeTe contents, the defect layers again lead to domain structures. In these cases, the cation defect layers (with van der Waals and partially covalent Te-Te bonding) can be viewed as boundaries between rhombohedrally distorted GeTe-like twin domains. These microstructures are due to the very long diffusion pathways that would be necessary to reach the stable superstructure with regularly spaced parallel van der Waals gaps. The influence of both the stoichiometry and the annealing-quenching process on the microstructure is very pronounced and can be tuned well. Its effect on thermoelectric properties will also be discussed.

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Resonant diffraction study of concentration gradients in multinary antimony tellurides. Matthias N. Schneider, Felix Fahrnbauer, Oliver Oeckler. *Department of Chemistry, LMU Munich, Germany.*
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In recent years, multinary antimony tellurides have gained interest as promising candidates for thermoelectrics and phase-change materials for data storage media. [1] Long-periodically ordered layered phases $(\text{MTe})_n(\text{Sb}_2\text{Te}_3)_m$, $(\text{Sb}_2\text{Te}_3)_m(\text{Sb}_2)_k$ and $(\text{MTe})_n(\text{Sb}_2\text{Te}_3)_m(\text{Sb}_2)_k$ ($M = \text{Ge}, \text{Sn}$) can be obtained by quenching and subsequent temperature treatment. They exhibit distorted rocksalt-type as well as A7-type building blocks as described for example for $9P\text{-GeSb}_4\text{Te}_4$ ($P\text{-}3m1$) or $51R\text{-Ge}_{2-x}\text{Sb}_{2+x}\text{Te}_5\text{Sb}_8$ ($x = 0.43$; $R\text{-}3m$). [2] $39R\text{-(Ge}_x\text{Sb}_{1-x})_2\text{Te}_3[(\text{GeTe})_y\text{Sb}_{1-2y}]_8$ ($x = 0.31$, $y = 0.033$; $R\text{-}3m$, $a = 4.266$, $c = 75.02$ Å) and $39R\text{-(Sn}_x\text{Sb}_{1-x})_2\text{Te}_3[(\text{SnTe})_y\text{Sb}_{1-2y}]_8$ ($x \approx 0.3$, $y \approx 0.03$; $R\text{-}3m$, $a = 4.292$, $c = 75.58$ Å), however, exhibit concentration modulations along the stacking direction, as shown by STEM-HAADF