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IAP-SEMINAR

EINLADUNG

Termin: **Dienstag, 17.11.2009 um 16:00 Uhr**
Ort: **Technische Universität Wien,**
Institut für Allgemeine Physik,
Seminarraum 134A, Turm B (gelbe Leitfarbe), 5. OG
1040 Wien, Wiedner Hauptstraße 8-10

Vortragender: **Prof. Dr. Dr. h.c. Stan Veprek**
Department of Chemistry, Technical University Munich, Garching/D

Thema: **The Search for Superhard Materials: Go Nano!**

Kurzfassung

Intrinsically super- (H ≥ 40 GPa) and ultrahard (H ≥ 80 GPa) materials attain high hardness from their large intrinsic strength, whereas extrinsically super- and ultrahard materials reach such hardness due to their nanostructure [1]. I shall discuss examples of bulk materials with high elastic moduli but relatively low hardness, because, upon shear strain, the materials undergo instability of the electronic structure and softening. Afterwards, I'll concentrate on the understanding of the origin of ultrahardness in nc-TiN/a-Si_3N_4 and related nanocomposites, in which 3-4 nm small TiN nanocrystals are "glued" together by about 1 monolayer thick SiN_x interface, that is strengthened by enhanced valence charge density. *Ab initio* DFT calculation of the shear strength of the interfaces, Sachs averaging, pressure enhancement of the flow stress and Tabor's relation between the hardness H and yield strength Y, $H \approx 2.84 \cdot Y$, explain why these materials can reach hardness significantly larger than diamond [2]. The charge transfer to the SiN_x interface induces Friedel oscillations of the valence charge density causing that ideal shear and decohesion to occur within the TiN nanocrystals but not in the SiN_xinterface [3]. Non-linear finite element modelling explains the unusual combination of mechanical properties of these materials [4]. Present industrial applications will be briefly discussed [5].

[1] S. Veprek, J. Vac. Sci. Technol. A **17** (1999) 2401
[2] S. Veprek et al., Phil. Mag. Lett. **87** (2007) 955.
[3] R. F. Zhang et al., Phys. Rev. Lett. **102** (2009) 015503; Phys. Rev. B **79** (2009) 245426.
[4] M. G. J. Veprek-Heijman et al., Surf. Coat. Technol. **203** (2009) 3385.
[5] S. Veprek and M. G. J. Veprek-Heijman, Surf. Coat. Technol. **202** (2008) 5063.

Alle interessierten Kolleginnen und Kollegen sind zu diesem Seminar
(45 min mit anschließender gemeinsamer Diskussion) herzlich eingeladen.

H. Störi e.h.
(LVA-Leiter)