DS 9: Hard Coatings II

Time: Monday 15:15–17:00 Location: H34

DS 9.1 Mon 15:15 H34

High Quality Cubic Boron Nitride Films - A Starting Point for Doping Experiments — •Hong Yin[1], Ivan Pongrac[1], Xuyang Wang[1], Hans-Gerd Boyen[1], Paul Ziemann[1], Bastien Dohuard[2], Laurent Houssiau[2], and Carla Bittencourt[3] — [1]Institute of Solid State Physics, University of Ulm, D-89081 Ulm, Germany — [2]LISE, University of Namur, B-5000 Namur, Belgium — [3]Materia Nova, B-7000 Mons, Belgium

After the successful demonstration that c-BN films can be epitaxially grown at 900°C on top of (001)-oriented diamond substrates [1], such high quality samples serve as starting point for their doping with Si atoms. For this purpose, a small stripe of a Si-wafer is co-sputtered during the c-BN deposition and the resulting concentration of Si as well as of unintentionally incorporated contaminants are determined by XPS, AES for near surface concentrations and ToF-SIMS for depth profiling. These results will be related to first temperature-dependent resistance measurements.

[1] X.W. Zhang, H.-G. Boyen, N. Deyneka, P. Ziemann, F. Banhart, M. Schreck, Nature Materials 4 (2003) 312.

DS 9.2 Mon 15:30 H34

Residual Stress in Nanocrystalline Diamond Films — •Nicolas Woehrl and Volker Buck — Thin Film Technology Group FB 7, University of Duisburg-Essen, Universitaetsstr. 3-5, 45141 Essen, Germany

Nanocrystalline films were deposited by microwave-plasma CVD at a pressure of 200 mbar from an $Ar/H_2/CH_4$ plasma where the hydrogen fraction in the process gas was varied between 2 and 7 %. Residual stress is a critical parameter in thin film deposition and especially important for technical applications of nanocrystalline diamond because high residual stress can lead to cracking or even to delamination of the film from the substrate. An ex-situ optical device was used to measure the residual stress of the substrate. It is shown that by controlling the process parameters the residual stress in the NCD films can be adjusted in a wide range even from compressive to tensile. The films were characterized by two wavelength scanning micro Raman spectroscopy and SEM. In this work a correlation is made between the intrinsic stress measurements and the Transpolyacetylene peaks (around 1120 cm^{-1} and 1450 cm^{-1}) in the Raman spectra of NCD films. It is shown that the intensity and the FWHM of the peaks correlate with the tensile stress in the films. A model correlating the Raman spectra to the grain size and thus to the intrinsic stress measurements is given in this paper.

DS 9.3 Mon 15:45 H34

Kinetic modeling of BN deposition by PECVD — •Sarah Panowitz, Jens Matheis, and Achim Lunk — Institut für Plasmaforschung, Universität Stuttgart, Pfaffenwaldring 31, D-70569 Stuttgart

We present kinetic modeling of BN deposition by PECVD in the system B-N-H-X where X represents the gases F, Cl, Br or O, respectively. In the first step the thermodynamic data as well as kinetic coefficients are collected from literature and compared with each others. The kinetic coefficients also include the most important plasma reactions. With data set up selected calculations were performed in the program "CHEMKIN". Kinetic modeling was executed with the perfectly stirred reactor model. This model requires modeling of volume reactions as well as reactions on the surface. The rate coefficients for the surface reactions are investigated through parameter studies. Results of these parameter studies are compared with data known from experiments to obtain the probably way of reaction mechanisms. Data from kinetic modeling are also compared with results from calculations in thermodynamic equilibrium. Results of kinetic and equilibrium modeling show that the range where BN can be deposited is very sensitive to the mole fraction of the species X which is used. Using oxygen as well as fluorine there exist only few parameter compositions to deposit BN. These parameter sets are very important in relation to possible etching effects in PECVD of c-BN deposition.

DS 9.4 Mon 16:00 H34

Correlation of structural properties of DLC films to their mechanical and optical properties — •Oleksiy Filipov, Alexei Poukhovoi, Nicolas Woehrl, and Volker Buck — Thin Film Technology Group, Dept. of Physics, University of Duisburg-Essen, Universitätsstr. 3-5, 45141 Essen, Germany

Diamond-like carbon films refers to a form of amorphous carbon a-C and hydrogenated amorphous carbon a-C:H containing a sizeable fraction of sp3 bonding, which makes them mechanically hard, infrared transparent and chemically inert. But DLC films have a big drawback high residual stress. In order to adjust stress and investigate properties of deposited films, DLC films were deposited onto different types of substrates like glass to investigate optical properties, Si and steel to investigate structural and mechanical properties, by using different deposition methods such as PVD DC-anodic arc and CVD RF-plasma. Both deposition methods allow us independently adjust substrate bias and gas admixture in order to influence the film properties. The structural properties of the films were characterized by Raman and FTIR spectroscopies. The optical properties of the films were ex-situ examined by UV-IR spectroscopy. The intrinsic stress was measured ex-situ by determining the substrate curvature using SSIOD method. It was shown correlation between structural and optical properties of deposited films and influence of deposition parameters onto intrinsic stress. The influence of hydrogen flow rate on film properties was also shown.

DS 9.5 Mon 16:15 H34

Electronic properties of graphite-like ion tracks in insulating tetrahedral amorphous carbon — Anne-Katrin Nix[1], Daniel Schwen[1], Carsten Ronning[1], Johann Krauser[2], Christina Trautmann[3], and •Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Hochschule Harz, Friedrichstrasse 57-59, 38855 Wernigerode, Germany — [3]Gesellschaft für Schwerionenforschung, Planckstrasse 1, 64291 Darmstadt, Germany

We investigated the formation of quasi one-dimensional conducting filaments in diamond like carbon (DLC) films created by swift heavy ion irradiation. Various DLC films with thicknesses of about 100 nm were grown using mass separated ion beam deposition (MSIBD) on highly conducting Si and Ni substrates. After deposition the films were irradiated with 1 GeV ^{238}U ions with fluences between 10^9 and 10^{11} ions/cm^2. Due to their high electronic energy loss of about 30 keV/nm the swift heavy ions graphitize the predominantly (80 %) sp^3-bound carbon film along their trajectories yielding conducting nanowires embedded in an insulating matrix. Using atomic force microscopy (AFM) with conducting cantilevers and applied bias voltage the presence of conducting tracks was confirmed and their conductivities were determined to be several orders of magnitude higher than of the host matrix. Temperature dependent electrical measurements were performed on the irradiated samples at 300 K - 10 K with fields up to 5 V/μm. We will discuss the results with respect to contact resistances and possible one-dimensional conduction mechanisms within the tracks.

DS 9.6 Mon 16:30 H34

Synthesis of MAX Functional Coatings by PLD — •Peter Schaaf[1], Christian Lange[1], Salvatore Cusenza[1], and Michel Barsoum[2] — [1]Universität Göttingen, II.Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Drexel University, Department of Materials Science and Engineering, Philadelphia, PA, USA

MAX phases - short for $M_{n+1}AX_n$ - constitute an exciting new class of materials. The prototype of this material class, Ti_3SiC_2, was first discovered and characterized in 1967 [1], but only in 1996 it was discovered that this material is stiff, lightweight, machinable, made from relatively inexpensive raw materials, resistant to oxidation and thermal shock, and capable of remaining strong up to temperatures in excess of 1300°C in air [2,3]. Since then, many MAX phases have been synthesized and characterized and first industrial applications occur [3]. Nevertheless, the potential of this material as a protective coating is not yet exploited. We report on experiments on the deposition of MAX coatings by PLD. The films were deposited at increasing substrate temperatures and subsequently analyzed by a variety of methods. Results on MAX coatings in the Ti-Si-C and the Ti-Al-N regime are reported.

[1] W Jeitschko and H Nowotny. 1967. Monatschrift für Chemie

98:329-337.
[2] MW Barsoum and T El-Raghy. 1996. Journal of the American Ceramic Society 79:1953-1956.
[3] MW Barsoum and T El-Raghy, American Scientist 89, 334 (2001).

DS 9.7 Mon 16:45 H34

An empirical bond-order potential for simulating amorphous (hydro)carbon film formation — •Lars Pastewka[1] and Michael Moseler[1,2] — [1]Fraunhofer Institut Werkstoffmechanik, Wöhlerstraße 11, 79108 Freiburg — [2]Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg

Process simulation, and especially the modeling of amorphous carbon and hydrocarbon thin film formation, has been of scientific interest for decades. The length and time scales which have to be covered for meaningful simulations are, however, still out of reach for quantum simulation techniques. Only quite recently insight has been gained into thin film formation using empirical potentials [1,2]. Available empirical potentials on the other hand have their own deficiencies: They either fail to describe carbon hybridization correctly, do not include hydrogen interaction, or if reliable are still too expensive. Here we present a straighforward extension of the carbon potential of Erhart and Albe [3] building on the original ideas of Brenner [4]. By utilizing an extended fitting database our potential manages to describe hybridization correctly while not sacrificing execution speed. This enables large scale studies of hydrocarbon thin film formation.

[1] M. Moseler et al., Science 209, 1545 (2005) [2] H. U. Jäger and K. Albe, J. Appl. Phys. 88, 1129 (2000) [3] P. Erhart and K. Albe, Phys. Rev. B 71, 035211 (2005) [4] D. W. Brenner, Phys. Rev. B 42, 9458 (1990)