INTERFACE STRUCTURE IN TiN/SiC NANOCOMPOSITES

Ivashchenko V.I., Scrynskyy P.L., Kuzmichev A.I., Ivashchenko L.A., Butenko O.O., Timofeeva I.I., Gran'ko V.M.
Institute for Problems of Material Science, NAS of Ukraine (Dep. 7),
Krzhyzhanovsky str. 3, 0380 Kyiv-142, Ukraine, e-mail: ivash@ipms.kiev.ua

Extended experience in the design of super-hard nanocomposites and understanding of their properties has been achieved during the last decade. TiN/SiN_x nano-composites are the most studied systems [1]. The strong increase in hardness as compared with pure TiN has been attributed to the nanometer scale randomly oriented TiN grains and one monolayer thick (1 ML) SiN_x interfacial layer [1]. The TiN/SiC hetero-structures have been studied to a lesser extent. Kong, Dai, Lao *et al*. have deposited nanolayered TiN/SiC coatings at room temperature [2]. They showed that the 3C-SiC layers have crystallized and grown with TiN layers in the (111) growth orientation.

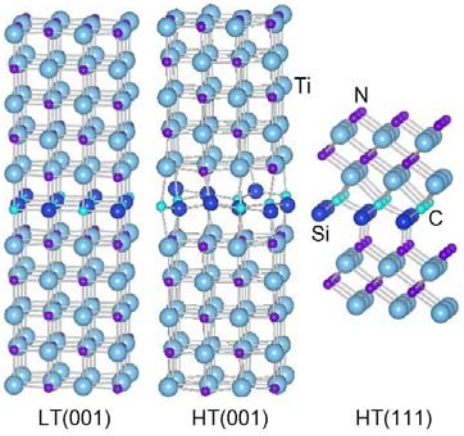

Fig.1. Atomic configuration of the low- (LT) and high-temperature (HT) TiN/1 ML SiC/TiN hetero-structures

In this work, we investigate the hetero-structures with one monolayer of interfacial SiC inserted between several B1(NaCl)-TiN (001) and (111) monolayers in the temperature range of 0-1400 K using first-principles quantum molecular dynamics (QMD) simulations. The temperature-dependent QMD calculations in combination with subsequent variable-cell structural relaxation reveal that the TiN(001)/B1-SiC/TiN(001) interface exists as pseudo-morphic B1-SiC layer at 0 K and 600 K (LT(001), cf. Fig. 1). After heating to 900-1400 K and subsequent static relaxation (HT(001)), the interfacial layer corresponds to a strongly distorted 3C-SiC-like structure oriented in the (111) direction in which the Si and C atoms are located in the same interfacial plane (cf. Fig. 1). The Si atoms form the four-fold Si-C_3N_1 coordinated configurations, whereas the C atoms are located in the C-Si_3Ti_2 surrounding.

All the (111) interfaces simulated at 0, 300 (LT(111)) and 1400 K (HT(111)) have the same atomic configurations. For these interfaces, the Si and C layers are similar to those that are aligned perpendicularly to the (111) direction in 3C-SiC. The Si and C atoms are located in Si-C_3N_1 and C-Si_3Ti_6 configurations, respectively.

The B1-SiC $\rightarrow$ 3C-SiC transformation at the interface of TiN/SiC nanocomposites above 600 K is confirmed with the XRD spectra of the nanolayered TiN/SiC coatings, presented in Fig. 2. We have deposited these coatings by dual magnetron sputtering the TiN and SiC target at different temperatures (T_S). It is clearly seen that the intensity of the SiC reflex at 2θ~35.6° jumps for the coating deposited at T_S above 600 K, in agreement with the results of our calculations.

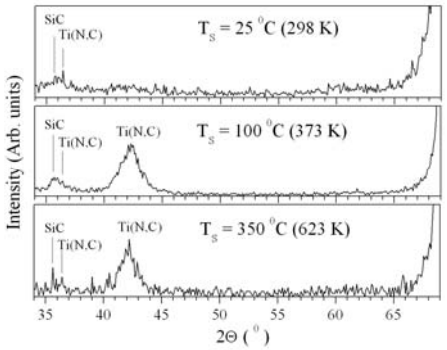

Fig. 2. XRD spectra of TiN/SiC nanolayered coatings. T_S is substrate temperature

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1. S. Veprek, A. Niederhofer, K. Moto, T. Bolom, H.-D. Männling, P. Nesladek, G. Dollinger, A. Bergmaier, Surf. Coat. Technol. **133-134**, 152 (2000).
2. M. Kong, J. Dai, J. Lao, G. Li, Appl. Surf. Sci. **253**, 4734 (2007).