

Effect of Laminating Period of Ceramics Superlattice Coating Film on Its Mechanical Properties

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Background

Ceramics superlattice, which has a laminated structure of heterogeneous ceramics combination in nanometric scale, is one of the most promising approaches as a highly functional coating film. As the ceramics superlattice shows high indentation hardness and thermal stability, it is expected to use as a wear-resistant coating films on the surfaces subjected to severe frictional contact such as cutting tools and slide ways. For example, it is reported that TiN/VN epitaxial monocrystalline superlattice film shows remarkable hardness enhancement [1]. The indentation hardness of the superlattice film depends on its laminating period and reaches the maximum value of $H_V = 55$ GPa at the period of 5.2 nm. This value corresponds to the hardness of more than twice as high as that of TiN or VN homogeneous films. Polycrystalline TiN/AlN superlattice film also shows the maximum hardness of 40 GPa at the period of 2.5 nm [2][3]. This value is approximately 1.6 times as high as that of TiN homogeneous film. However, the mechanism of hardness enhancement has not been understood well due to the difficulties in highly reliable measurement of mechanical properties and observation of microstructure of the superlattice film.

In this paper, to clarify the correlation between laminating period and mechanical properties of ceramics superlattice and to establish the guidelines for design of highly functional superlattice coating films, molecular dynamics (MD) computer simulations of uniaxial compression testing are carried out on TiN/ZrN superlattice films with various laminating periods.

MD modeling of ceramics superlattice

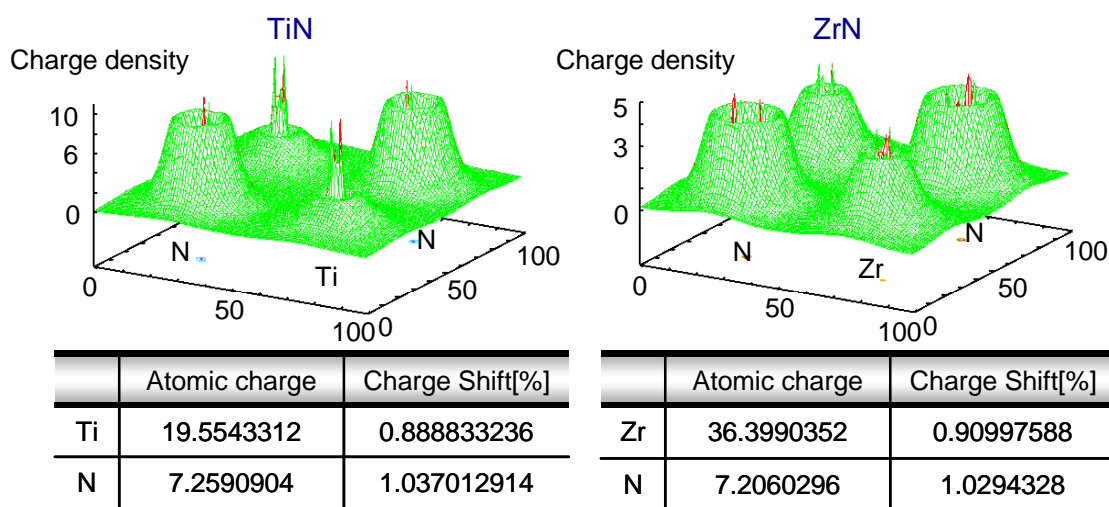


Fig.1 First-principle calculation of electronic charge density distribution in TiN and ZrN

MD simulation is an useful method to analyze accurately the atomistic behavior of the deformation or fracture process of an atomic solid model. For the analysis, three-dimensional (3-D) TiN/ZrN superlattice model with various laminating periods are used assuming the interatomic potential functions based on the modified embedded atom method (MEAM) [4]. Figure 1 shows electric charge density distribution of TiN and ZrN calculated by the use of a full potential linearized augmented plane wave package for calculating crystal properties (WIEN97) [5]. The MEAM potential parameters regarding electric charge density distribution are determined by fitting the density distribution between N and Ti and Zr with that of the calculated distribution of valence electrons. The other parameters are determined by fitting the cohesive energy, elastic modulus, atomic volume and interatomic distance with those of measured values.

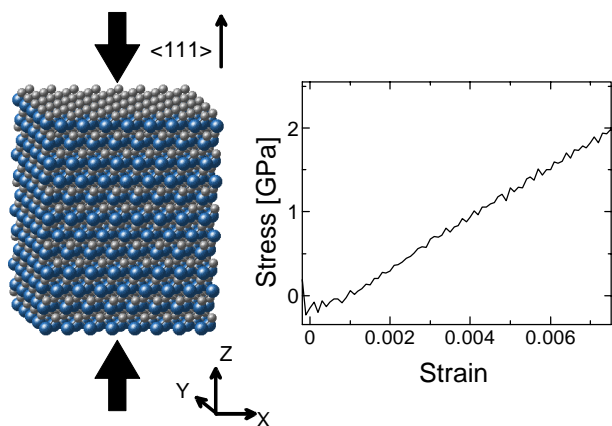
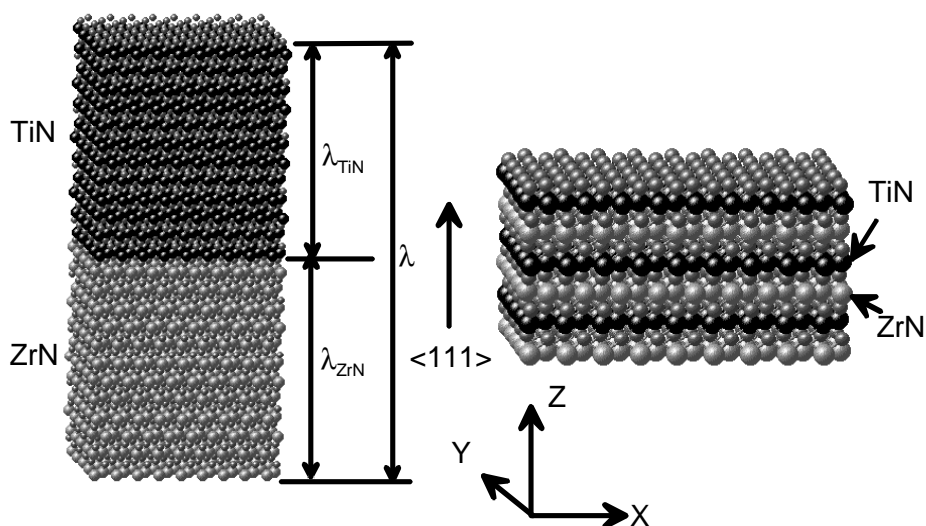


Fig.2 Uniaxial compression testing for TiN and ZrN

To analyze the deformation behavior of monocrystalline TiN and ZrN, MD simulation of uniaxial compression testing are carried out using 3-D model as shown in Fig. 2. Both of TiN and ZrN models have (111) top plane in z-direction and periodic boundaries are applied in x, y and z-directions. Young's modulus is calculated from the stress-strain curve when the model is compressed in z-direction. The Young's modulus of TiN and ZrN obtained from the simulations are 340 GPa and 390 GPa, respectively, which are 10-15 % smaller than those of measured values.

Figure 3(a) shows the MD model of TiN/ZrN superlattice for uniaxial compression testing. The thin layers of TiN and ZrN with same thickness are alternately laminated in <111> direction. The laminating periods of the models used in the simulation are 1.5, 3.0 and 6.1 nm. In addition, the monolayer-laminating model (Ti/N/Zr/N/Ti/N/Zr/N----) is also used as the model of an extremely



(a) Laminating period
 $\lambda = 1.5, 3.0, 6.1 \text{ nm}$
 $(\lambda_{\text{TiN}} : \lambda_{\text{ZrN}} = 1:1)$

(b) Monolayer laminating

Fig.3 Uniaxial compression testing for TiN/ZrN superlattice

small laminating period, as shown in Fig. 3(b). The initial interatomic distance between N and Ti and Zr is set to be the average value of those in monocrystalline TiN and ZrN homogeneous films.

Strain distribution in the MD models of superlattice at stable state after relaxation show that compressive and tensile strain are stored in the layer of ZrN and TiN, respectively, and that the maximum strain level and uniformity of distribution are increases as the laminating period decreases.

Effect of laminating period on mechanical properties

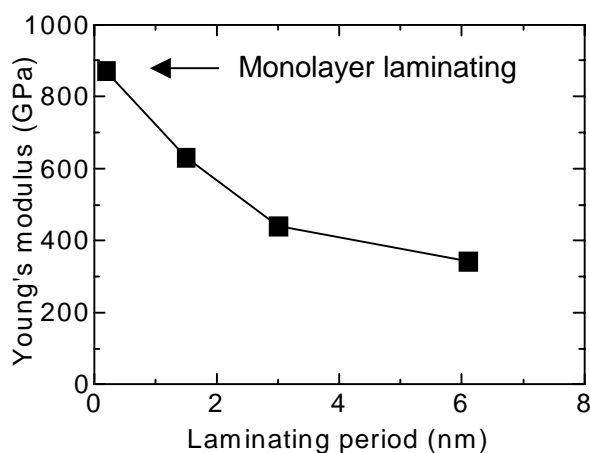


Fig.4 Effect of laminating period on Young's modulus (simulated)

MD simulations of uniaxial compression testing show that the Young's modulus of TiN/ZrN superlattice increases as the laminating period decreases, as shown in Fig. 4. When the laminating period is 6.1 nm, Young's modulus of superlattice is almost same as that of monocrystalline TiN and ZrN homogeneous films. However, it increases to 1.6 times as high as that of homogeneous films at the laminating period of 1.5 nm. In case of monolayer-laminating superlattice, Young's modulus is enhanced to 2.3 times as high as that of homogeneous films.

On the other hand, Fig. 5 shows the results of Knoop hardness testing of practical TiN/ZrN superlattice coating films with various laminating period. The

superlattice films, the thickness of which is about 2.5 μm , are deposited on cemented carbide substrates using an arc ion plating method. The laminating period is controlled by the rotation speed of substrate holder and arc current [3]. The indentation hardness increases as the laminating period decreases as is seen in the results of simulation in Fig.4. The hardness is enhanced to about 1.5 times as high as that of homogeneous films at laminating period smaller than 1.6 nm. Both of the results of simulation and experiment qualitatively show the same tendency that higher mechanical properties are observed on the films with smaller laminating periods. While Young's modulus is a measure or

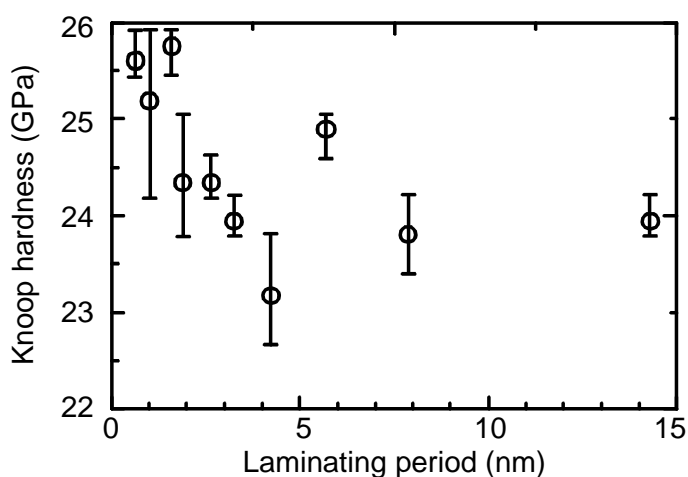


Fig.5 Effect of laminating period on indentation hardness (measured)

indicator of the strength of resistance to elastic deformation, indentation hardness is that to plastic deformation. Hence, it is difficult to directly compare the effect of laminating period on the enhancement of Young's modulus with that of indentation hardness. However, from atomistic point of view, mechanical properties of a material are essentially depending on interatomic potential between the atoms composing the material. In case of ceramics superlattice, large curvature of interatomic potential function in the region near the equilibrium interatomic distance results in the enhancement of both of Young's modulus and indentation hardness. MD simulations of indentation and scratching on ceramics superlattice films are now under consideration.

For the qualitative discussion about the effect of laminating period on the strength enhancement, difference in microstructure should be taken into account between the MD models and practical coating films. As the practical coating films have polycrystalline structure, atomic misfits and grain boundaries are inevitably included in the film. The defects included in the film may deteriorate its mechanical properties. Further simulations on the model including defects are now being continued.

Conclusions

To clarify the mechanism of hardness enhancement, MD simulations of uniaxial compressive testing of TiN/ZrN superlattice coating films with various laminating period are carried out. The results show that Young's modulus of the film increases as the laminating period decreases. In case of monolayer-laminating superlattice, Young's modulus is enhanced to 2.3 times as high as that of homogeneous films. The results of Knoop hardness testing on practical TiN/ZrN superlattice coating films with various laminating period shows the same tendency as is seen in the relation between laminating period and Young's modulus obtained from the simulations. MD simulation can be a useful tool for profound understanding of the correlation between microstructure and mechanical properties and for establishing the guidelines for the design of highly functional ceramics superlattice coating films.

Acknowledgements

This work was supported by the Grant-in-Aid for Scientific Research (B2) (12450059) of the Ministry of Education, Science, Sports and Culture, Japan and Osawa Scientific Studies Grant Foundation. The authors express their thanks to Mr. M. Setoyama, Engineering Department, Nippon ITF, Inc. and Mr. H. Fukui, Itami Laboratories, Sumitomo Electric Industries, Ltd. for supplying the superlattice specimens and hardness measurement and Messers. M. Tsurutani and K. Yuki for their cooperation in simulation.

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