Supplementary Materials

Deformation behavior of hard ceramic layer coated Ti composite: *in situ* characterization and molecular dynamics simulation

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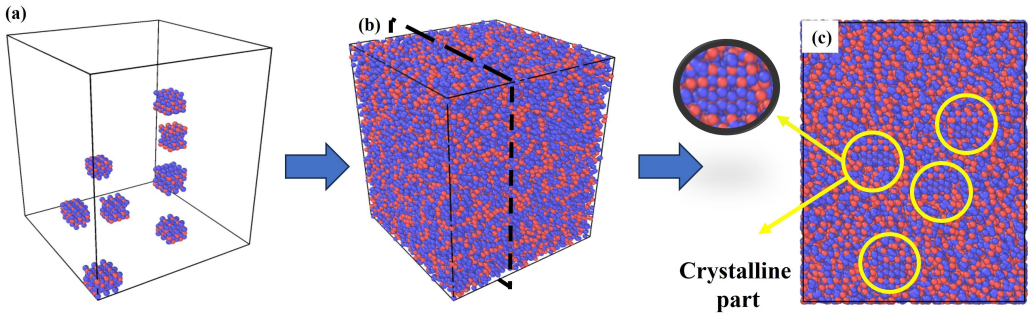

Fig. S1. (a, b) the spatial distribution of the crystal part in the model; (c) the cross-sectional position in (b)

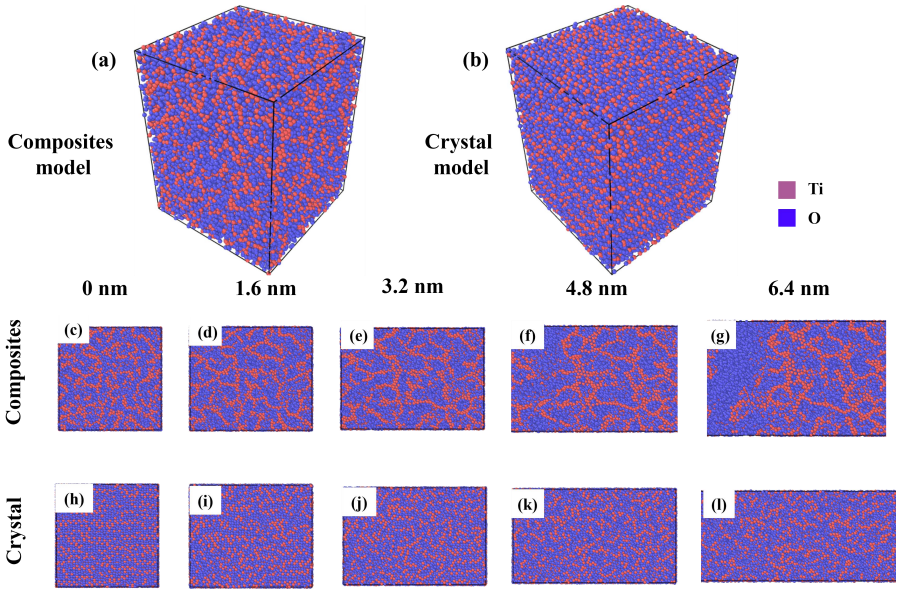

Fig S2 (a, b) the crystal/amorphous dual phase composite structure and crystal TiO_2 model. (c-g) the simulation of composite structure, (h-l) the crystalline TiO_2 structure

Fig.S1 shows the modeling process of the crystal/amorphous hybrid structure, and the position of the crystalline part in the amorphous TiO_2 structure. Figs.S2(a, b) shows the two models of the composite structure and crystal structure, and Figs.S2(c-l) show the simulation results of the hybrid model of crystal/amorphous hybrid structure and single crystalline structure. Among the hybrid structure, the crystalline and amorphous portions are modeled according to different volume ratios. Fig.S3 shows the stress-strain curves obtained from the LAMMPS tensile simulation for the models with different volume ratios, which provides an important basis for the quantitative analysis of the coating properties.

Fig. S3 shows the molecular dynamics simulation results of different types of coatings attached to titanium substrates, including the following parts: (a, b) shows the crystal/amorphous two-phase composite structure and its pure titanium substrate model attached to crystalline TiO_2. (c-h) shows the simulation results of crystal amorphous coating attached to titanium substrate. (i-n) shows the simulation results of amorphous coating attached to titanium substrate. These figures demonstrate the adhesion behavior and structural characteristics of different coatings on titanium substrates. By comparing these simulation results, the influence of coating structure on the adhesion performance of titanium substrate can be analyzed, especially the behavior under different combinations of crystalline and amorphous phases.

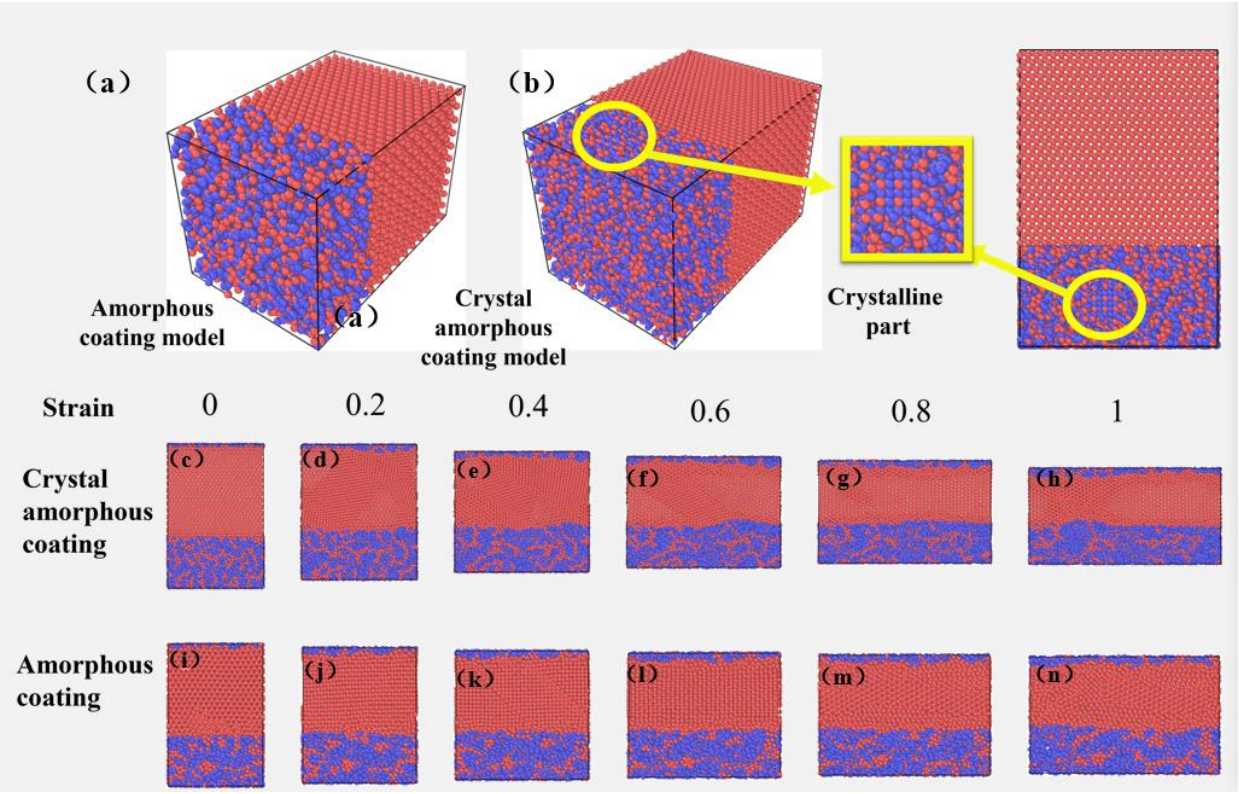

Fig. S3 (a, b) shows the crystal/amorphous biphasic composite structure and the model of pure titanium substrate attached to crystalline TiO_2; (c-h) Crystal amorphous coating attached to titanium substrate simulation; (i-n) amorphous coating attached to titanium substrate simulation

As shown in Fig.S4, it can be found that the tensile strength of the coating increases slightly with the increase of crystalline TiO_2 content. Specifically, the increase in amorphous TiO_2 content makes the coating more susceptible to damage under the tensile stress, and the damage occurs preferentially in the amorphous region. This phenomenon illustrates the effect of amorphous composition on the tensile properties of the coating. As for PEO and PEO-MH coating, the tensile strength of the PEO coating is relatively lower than that of the PEO-MH coating, which is attributed to the higher amorphous TiO_2 content in the PEO coating.

These simulation results are in agreement with the experimental results, further validating the conclusion that the overall tensile strength of the PEO-MH coating is higher than that of the PEO coating. This agreement not only confirms the validity of the simulation method, but also provides an important reference for coating design and optimization.

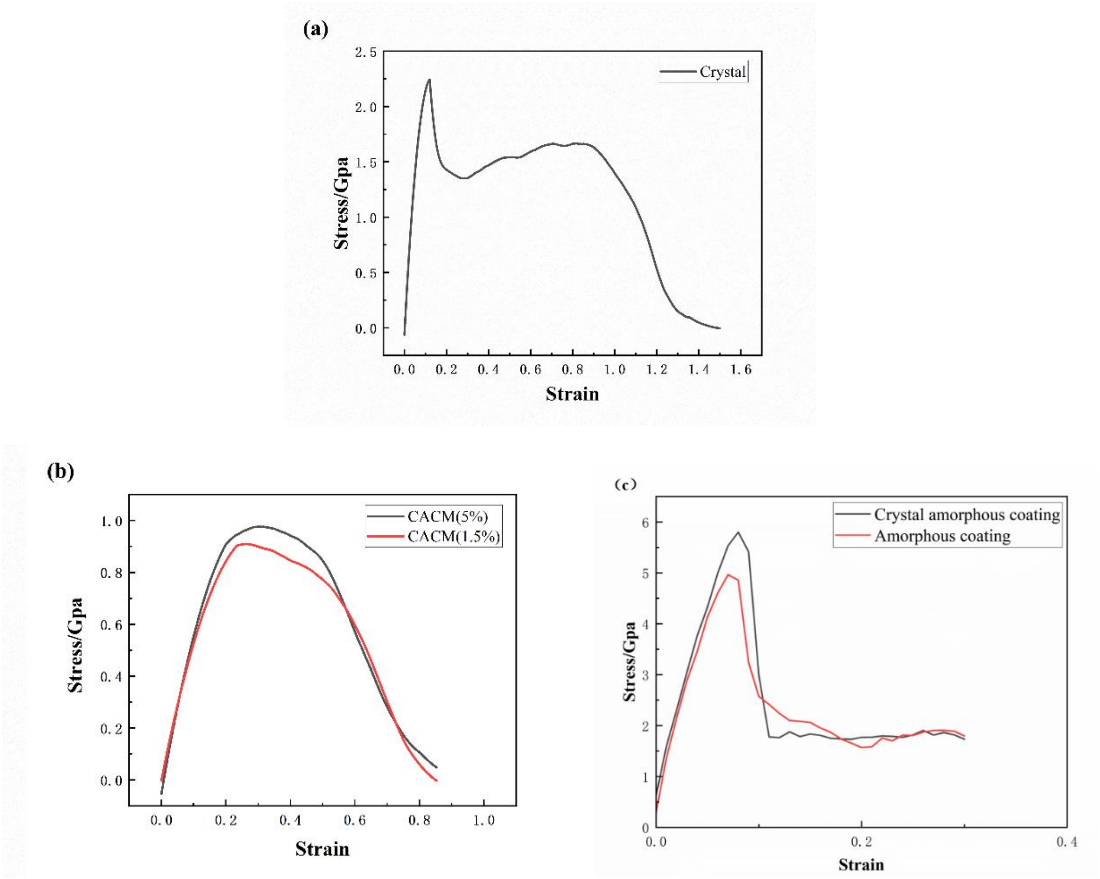

Fig. S4 Molecular dynamics simulation stress-strain curves; (a) Simulation results of the anatase TiO_2 crystal model; (b) Simulation results of the mixed model with 5% and 1.5% crystalline content.(c) Simulation of tensile curves of amorphous coating attached to titanium substrate and crystalline amorphous coating attached to titanium substrate.