Contribution ID: **136** Type: **Poster**

Microscopic Mechanism of Mg-Al Alloy Coating Damping Properties：A Molecular Dynamics study

Tuesday 19 June 2018 18:00 (20 minutes)

With the rapidly development of science and technology in modern industry, the failure of mechanical parts caused by mechanical vibration become one of the main factors of affecting mechanical performance. Hard coatings, such as metallic and ceramic coatings, were reported the outstanding damping potential by the experience. Among them, Mg-Al alloy coating was widely used due to excellent corrosion resistance and damping property. Although, it is observed that microstructures can lead to complex damping characteristics through microscopic characterization and damping tests, the mechanism of their damping mechanisms is not understood clearly, especially the effect of various microstructures on their damping properties.
Studies showed that the coating's damping characteristics are closely related on its internal microstructure, especially within the coating of micro-defects. However, the methods of experimental research will inevitably introduce other variables result in affecting the experimental results. In addition, Mg-Al alloy coating will form dislocations due to the crystal structure, preparation methods and process technology and other reasons. It has effect on the damping and mechanical properties. The use of computer simulation method avoid the above problems effectively .Meanwhile, the microscopic defect scale is the nanometer level, which is difficult studied by the experience. The molecular dynamics simulation method is used to explore the effect of microscopic defects on the damping performance of the coating, which lays the foundation for the study of coating deformation and failure mechanism.
In this paper, molecular dynamics simulation method is used to analyze the mechanical properties and damping mechanism of Mg-Al alloy coating. The molecular dynamics model of different types of Mg-Al alloy coating are obtained by modeling and simulating a variety of microscopic defects such as dislocation .The stress - strain curve, the total strain energy(W), the distortion energy(△W) and the damping factor (Q-1) under different conditions can be obtained by applying the impact and cyclic stress respectively. The microstructure of the coating is analyzed by Ovito visualization software. Changing the temperature condition and applying a fixed impact to the model. The results are analyzed by curves, energy and damping parameters of the model at different temperatures. Exploring the factors of influencing the mechanical properties of the Mg-Al alloy coating and microscopic mechanism of damping.

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Session Classification: Poster Session Tuesday

Track Classification: Surface Science & Applied Surface Science