Adhesion Analysis of Electroless Ni Coating on SiC_p/Al Composite Mirror Substrate

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Abstract: SiC_p/Al composite, which has light mass, high thermal conductivity and strength, enhanced specific modulus, compatible coefficient of thermal expansion (CTE), sufficiently high wear resistance, is considered as a promising material for the space lightweight mirror. In order to improve the polishing properties of the material, electroless Ni plating on SiC_p/Al composite for the space lightweight mirror was carried out. The adhesion of the coating and substrate was also studied by experiments and molecular simulations. The morphologies of the coated layers were inspected by means of scanning electron microscope (SEM). The experimental results demonstrate that the coating is uniform and compact. The assessments of coatings adhesion were made using scratch test, and the critical load L_c is more than 100 N. Molecular dynamics (MD) was used to simulate the interactions of the coating and composite, and the calculated interaction energy is 108.4 $kJ\cdot mol^{-1}$.

Key words: SiC_p/Al composite; electroless Ni plating; adhesion analysis

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With the rapid development of the remote sensing technique, more and more requirements are needed in improving the ground resolution of the space optics. Many efforts focus on the research of high performance, low cost, very lightmass reflective telescope systems[1]. Aluminum matrix composites reinforced with SiC particles (SiC_p/Al) is a promising material available for optics mirrors because of its outstanding advantages, including light mass, high thermal conductivity and strength, enhanced specific modulus, compatible coefficient of thermal expansion (CTE), sufficiently high wear resistance, and so on[2]. Nevertheless, the polishing properties of the material are limitated due to stiffness of SiC. To solve this problem, the nickel is deposited on its surface by electroless plating, which provides distinct advantages, for instance, uniformity of deposits on complex shapes, low-cost, simple equipment as well as good characteristics involving high-temperature resistance, oxidation resistance, corrosion resistance and better ornamental performance. Electroless plating with catalytic metals is an effective way for necessary surface treatments. The coated layers can serve as a medium for the adhesion and transferring loads.

The first and foremost requirement for the application of coating techniques is that the deposited coatings should be well adhesive to the substrate[3,4]. This research is dealing with electroless Ni plating on SiC_p/Al composite for the space mirror and evaluating the adhesion of coatings and substrate materials. On the base of the experiments, the adhesion of electroless Ni coating on SiC_p/Al composite is analyzed with the software package Materials Studio (MS).

1 Experimental

The dual sized SiC particles with 20 μm and 60 μm were chosen to obtain a volume fraction of 70 %, because the volume fraction of identical particles was limited and usually lower than 64%. An Al alloy (4032Al), the compositions (wt%) of which were 12 % Si, (0.5~1.3)% Cu, (0.8~1.3)% Mg, 1.0% Fe, (0.5~1.3)% Ni, and Al balance, was used as the matrix. Aluminum matrix composites reinforced with 70%(volume) of SiC particles were fabricated by squeeze-casting technology. Radius of SiC_p/Al composite mirrors for electroless Ni plating was 5 cm.

Prior to being plated, the composites surfaces of any contaminants were cleaned by immersing them into the acetone solution for 8 min and 10 min activated in a $PdCl_2$ acidic solution. Then electroless Ni was deposited on the SiC_p/Al composite using an alkaline bath[5,6]. The

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solution was maintained at of 45 ℃ with a pH of 8.5.

The surface morphologies of the SiC_p/Al composite and coatings were inspected by scanning electron microscope (SEM, S-4700).

The assessments of coating adhesion were made using a scratch test instrument (WS2000, Lanzhou Institute of Chemical Physics, the Chinese Academy of Sciences) equipped with a 200 μm diameter, 120° cone angle diamond scratch indenter. The critical load L_c, the value at which the first failure occurs, was determined from the acoustic signal emitted during the scratching procedure, and SEM was also employed for the analysis of crack morphologies and for the examination of the mechanism leading to the coating delamination. The 6 mm long scratches produced in this way were then examined microscopically to estimate the load at which either the coating peeled off from the substrate or it was completely removed from the scratch channel.

2 Modeling and Computational Method

The nature of the adhesive interfaces between the coating and the substrate were studied by the method based on constant pressure molecular dynamics (MD) with the software package Materials Studio (MS).

MD simulations were routinely applied to study structure and dynamic behavior of molecules in their bulk and thin film states over the past few decades with considerable success[7]. As a kind of powerful theoretical methods, MD simulations could be used to calculate the mechanical properties[8]. To calculate the adhesion properties of the coating and SiC_p/Al composite material, MD method was used on the basis of the experimental determination. The modeling and computational details are as follows.

The lattice parameters of a=0.3078 nm, b=0.3078 nm, c=1.0460 nm, $\alpha=\beta=90^o$, $\gamma=120^o$ and the coordinates of the SiC structure with P63MC space group, the lattice parameters of $a=b=c$=0.4035 nm，$\alpha=\beta=\gamma=90^o$ and the coordinates of Al structure with FM-3M space group, and the lattice parameters of $a=b=c$=0.3525 nm，$\alpha=\beta=\gamma=90^o$ and the coordinates of Ni structure with FM-3M space group were taken from their XRD determine results [6]. There was a supercell of SiC (2×1×1) and Al (5×2×1) in the simulation box which constructed SiC_p/Al composite (the components of the material was properly simplified in the model). The density of SiC_p/Al compostie model was same as the mirror material (3.0 $g \cdot cm^{-3}$). Several fixing and relaxing steps were performed to keep the inner layers with a crystal-like structure. The coating model was assembled with a suprecell of Ni (4×8×1) surface slab, and the periodic boundary conditions were applied to simulate an infinite system.

MD simulations were carried out using MATERIALS STUDIO 3.0 software package (Accelrys Co.) The models were built with a Visualizer module, the molecular dynamics and the minimization calculations were performed on the Discover module. The force field we implemented in this work was COMPASS (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies), which was based on the earlier class II CFF9x and PCFF force fields and was the first ab initio-based force field that was parameterized using extensive data for molecules in the condensed phase. The MD simulations were performed within a canonical ensemble (NVT) at 298 K, and the temperature was controlled by Andersen method. The atom-based summation technique was employed to calculate the nonbonded interactions (van der Waals and electrostatic), with a cutoff radius of 1.55 nm. The total simulation time is $2\times10^5\times10^{-15}$ s, and the time step is 1×10^{-15} s. The trajectory information was recorded every 110×10^{-15} s. The substrate with the lowest energy was minimized using the cell-based summation method to compute the nonbonded interac- tions. The smart minimizer was employed, combining the steepest descents method and conjugate gradient method.

The interaction of Ni coating with SiC_p/Al composite that is, adhesion energy, was studied by molecular simulations.

3 Results and Discussion

Fig.1 and Fig.2 show the photographs and SEM morphologies of the coated SiC_p/Al composite mirror surface obtained after 3 h electroless plating. It can be seen from the images, the surface of the coating layer is compact, uniform, and smooth. There is no apparent flaw on the surface of the interlayer. The thickness of the interlayer is about 36 μm.

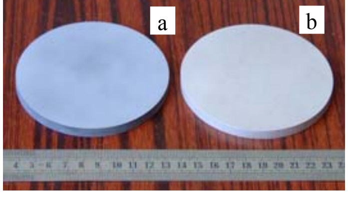

Fig.1 Photograph of samples before and after coating: (a) before coating; (b) after 3 h coating

The adhesion quality of the coating layer and the substrate is evaluated by scratch test. Fig.3 shows SEM micrograph taken from the 100 N load scratch. There is no evidence of the cracking at the coating- substrate interface. For this investigation, the nickel coatings remain adherent and there is no exposure of the substrate. With increasing of the applied load, there is no increase in the acoustic emissions produced during the scratching procedure. Therefore, the adhesion of the nickel to the SiC_p/Al composites is very good, as indicated by the high critical loads.

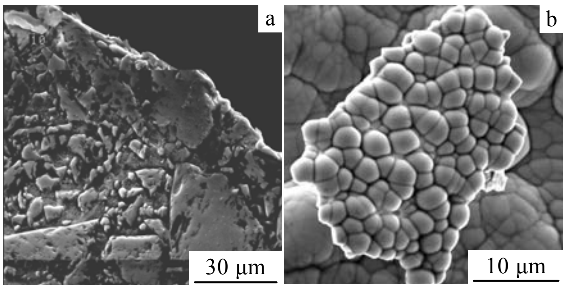

Fig.2 SEM micrographs of samples before and after coating: (a) before coating; (b) after 3 h coating

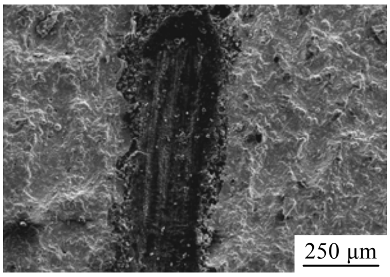

Fig.3 Scratch tests on Ni coatings

The structure model of the nickel-coated SiC_p/Al composite is obtained from Materials Studio, as shown in Fig.4.

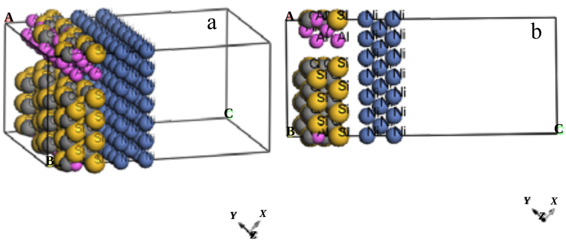

Fig.4 Structure model of electroless Ni plating on SiC_p/Al composite: (a) model of Ni-coated SiC_p/Al structure; (b) model of Ni-coated SiC_p/Al structure projected onto *XY* plane

Fig.5 shows snapshots of Ni coating and SiC_p/Al composite observed at 200 000 step of the simulation equilibrium. Initially, the coating is put regularly on SiC_p/Al composite surface in a distance of about 0.373 nm (see Fig.4). The simulations indicate that all nickel atoms would move toward the SiC_p/Al composite until they finally wrap on the surface of the substrate and the equilibrium is achieved.

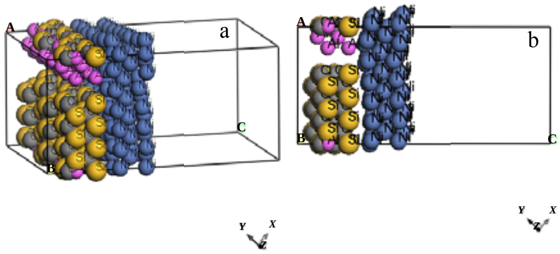

Fig.5 Configuration of electroless Ni plating on SiC_p/Al composite surface after MD equilibrium: (a) configuration after MD equilibrium; (b) configuration projected onto *XY* plane after MD equilibrium

Fig.6 shows the nonbond and potential energies during the simulation and it can be found that the energies of the system are stabile, indicating that the system attains to the equilibrium.

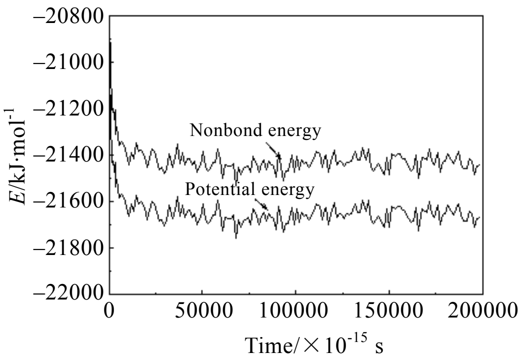

Fig.6 Energy vs simulation time

The dynamic behavior of nickel-coated SiC_p/Al composite can be illustrated by tracking the interaction energy of the system. Generally, the interaction energy is estimated from the difference between the potential energy of the whole system and the potential energies for the coating and corresponding SiC_p/Al composite as follows:

$$\Delta E=E_{total}-(E_{Ni}+E_{SiC_p/Al})$$

Where E_{total} is the total potential energy of the coated composite, E_{Ni} is the energy of the nickel coating without SiC_p/Al, and $E_{SiC_p/Al}$ is the energy of SiC_p/Al without the nickel coating. In other words, the interaction energy can be calculated as the difference between the minimum energy and the energy at an infinite separation of the nickel coating and SiC_p/Al matrix. The total interaction energies between Ni and SiC_p/Al are recorded every 1×10^{-12} s. Finally, the averages are calculated during the simulations. The interaction energy between the coated Ni and SiC_p/Al composite is 108.4 kJ·mol^{-1}. The results show that the attractive interaction between the simulated SiC_p/Al composite and the coating is stronger[9], which is in accord with experimental results.

4 Conclusion

The nickel layers can be coated onto SiC_p/Al composite by electroless plating method. SEM micrographs show that the continuous and complete coating layers can cover SiC_p/Al composite. The scratch tests and MD simulations can be used to investigate the interaction of the coating and SiC_p/Al composite. The adhesion energy plays an important role in the adhesive strength of the coating to the substrate. Combining the experimental results with the theoretical analysis, the adhesion state between the Ni coating and SiC_p/Al composite can be simulated and explained.

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SiC_p/Al 复合材料反射镜坯表面镀镍层的结合分析

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摘 要：SiC_p/Al 复合材料具有质量轻、导热性能好、高强度、高比模量、热膨胀系数低、耐磨损等优点，在空间轻型反射镜领域有良好的应用前景。在 SiC_p/Al 复合材料表面化学镀镍可以改善其抛光性能。本研究采用实验和分子模拟方法探讨了镀层与 SiC_p/Al 复合材料表面的结合机制。采用扫描电子显微镜观察镀层的表观形貌，结果表明，镀层均匀致密；采用划痕实验测试镀层的结合强度，其临界载荷 L_c 大于 100 N。同时，采用分子动力学模拟的方法从理论上分析镀层与基体的结合状态，并计算出二者的结合能为 108.4 kJ·mol^{-1}。

关键词：SiC_p/Al 复合材料；化学镀镍；结合分析

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