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La doping inhibits stress production at the grain boundaries in Ni–WC coating

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Abstract: Ni–WC–La₂O₃ wear-resistant coatings are prepared by a plasma spray method on the pure iron. The microstructure and wear resistance of the coating are investigated. After La₂O₃ doping, the wear resistance of modified coating was enhanced significantly. The amount of coating wear was reduced by 61.9% and the friction coefficient was reduced by 35.7% because of the La₂O₃ content of 1.5 wt.% compared with the Ni–WC coating. La₂O₃ can suppress WC precipitation along the grain boundaries, and reduce the number of cracks in the substrate near the WC phase. Furthermore, the diffusion and segregation behavior of La atoms is studied by first-principle calculation. The simulation results show that La doping can increase the bonding energy between the WC particles and the Ni substrate, consequently improve the abrasion properties of the coating. The cohesive energy of the interface is the smallest when the La atoms occupies Ni atomic sites of the interface, as result a stable Ni–WC interface is formed on the interface. A Ni–La amorphous transition layer is

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