Simulation and experiments on the performance of Co and Mo doped AgNi contact materials

Jingqin Wang¹, Jiying Jia¹, Defeng Cui², Peijian Guo³ and Ningyi Lu⁴

¹ State Key Laboratory for Reliability and Intelligentization of Electrical Equipment, Hebei University of Technology, Tianjin, People’s Republic of China
² Guilin Electric Appliance Research Institute Co. LTD, Guilin, People’s Republic of China
³ Tianjin Electric Science Research Institute Co. LTD, Tianjin, People’s Republic of China
⁴ Xiamen Hong Power Generation Sound Co., Ltd Testing center, Xiamen, People’s Republic of China

E-mail: jqwang@hebut.edu.cn

Keywords: AgNi, first principles, stability, powder metallurgy method, electrical contact performance

Abstract

In response to the inadequacy of experimental methods to explore the effect of doping modification on the performance of AgNi contact materials, the Ag/Ni interface simulation model was established based on the first-principles density functional theory to study the interfacial stability and electronic structure of Ag/Ni with Co-doped and Mo-doped. The stability at the interface can directly affect the anti-melt welding performance of AgNi contact materials. The doping can enhance the interfacial bonding stability of Ag/Ni, the hybridization of Ag and Ni orbitals and the bonding strength of Ag-Ni metal bonds, among which the Mo-doped AgNi has the best stability. The contact materials were prepared by powder metallurgy method. Wettability test and electrical contact performance test were conducted on AgNi contacts before and after doping. It was found that Co and Mo doping improved the anti-melt welding performance and anti-arc erosion performance of the intrinsic contact materials, which verified the simulation conclusions. The doping of Mo in AgNi contacts resulted in a substantial reduction of melt welding force and a significant reduction of material loss, which had the most obvious improvement effect on the contact materials.

With the increasing awareness of environmental protection and the promulgation of the EU RoHS directive, the ideal AgCdO contact materials will gradually be replaced by AgNi contact materials due to the toxicity of Cd [1]. Traditional AgNi electrical contact materials with good conductivity, heat conductivity and welding performance, low and stable contact resistance and processing performance advantages [2], are widely used in the contact resistance, the temperature requirements more stringent level of small and medium-sized current relay, contactor, micro switch, etc in the low voltage apparatus. However, in working current larger applications, the poor fusion welding resistance and electrical wear resistance of conventional AgNi materials limit the further popularization and application of AgNi materials [3, 4].

Literature research shows that doping modification can enhance the various properties of AgNi contact materials. Most scholars are currently based on powder metallurgy method, chemical reduction and liquid phase mechanical stirring method, powder mixing method and other experimental methods [5–9]. From the characterization of the test results, it can be concluded that doping can effectively improve the performance of AgNi material, while the microscopic mechanism and universality of the system cannot be analyzed in detail. There will be a series of problems such as long test cycles, a wide variety of doping elements, and blind test processes [10], so the method of computational research is introduced to explore the influence of metal doping on the performance of AgNi material, which can better understand the interaction between atoms from the microscopic level, avoid the blindness of experimental exploration, reduce energy waste and improve the research efficiency.

Reference [11] introduced a criterion for evaluating the dynamic fusion welding resistance of contact materials and their paired forms, based on which it was predicted that doping with Co and Mo could improve
the fusion welding resistance of AgNi contact materials, so Co and Mo were selected as doping elements in this study to investigate the effect of metal doping on the performance of AgNi contact materials. Reference [12] studied the contact materials of Ag-Ni-NiO doped with Co and found that the contact materials doped with Co had reduced contact engagement, contact wear, and material transfer, and improved the contact resistance to melt welding. Reference [13] found that metal Co-doped AgSnO\textsubscript{2} contact material can significantly improve the stability of the material, compared with undoped AgSnO\textsubscript{2}, its contact resistance, arc ignition energy, and material loss are reduced, and the microscopic morphology map after electrical contact test becomes flat. The refractory metal Mo is used as the doping element and suspended in the molten pool under the action of arc to increase the viscosity of the molten pool and improve the electrical wear resistance of the material [14], and it forms a brittle intermetallic compound with the reinforcing phase Ni, further enhancing the material brittleness and reducing the melt welding force, thus improving the anti-melt welding performance and electric wear resistance of the silver-nickel material.

In this paper, the metal-doped silver-nickel contact material was simulated and tested. The effect of doping on the stability of Ag/Ni interface and electronic structure was analyzed by simulation, and then the AgNi contact material was prepared by powder metallurgy method. Wettability and electrical contact performance was tested to verify the correctness of the simulation results, and then the doping of Co and Mo was comprehensively analyzed to improve the performance of AgNi contact.

1. Interface model and calculation method

1.1. Constructing the model
In view of the existing studies, among the bonding forms of Ag-Ni interface, Ag(110)/Ni(211) has the highest interfacial bonding energy, the most intense electronic hybridization at the interface and the most stable interfacial bonding [15], therefore, in this paper, the Ag/Ni interface model is constructed by combining Ag(110) and Ni(211) crystalline surfaces (figure 1(a)). The corresponding atomic layers (Ag: 8 layers, Ni: 6 layers) were selected through the convergence test of surface energy [16]. In order to eliminate the interaction between the upper and lower interface atoms, a 1.5 nm vacuum layer was added to the model. The UBER method was used to calculate and determine that the Ag/Ni interface spacing was 0.2 nm, and the system energy reached the minimum [17]. In the optimization process of the interface model, the atoms near the interface participate, which has little effect on the bottom atoms. Therefore, the four layers of Ag and three layers of Ni close to the Ag/Ni interface are allowed to relax freely in the geometric space, and the remaining atomic layers remain fixed to simulate the Ag/Ni interface structure. The doped atoms replace one of the free-relaxation Ni, and the different doping positions are numbered and marked red in figure 1(b).

1.2. Calculation method
In this paper, the Castep module in Material Studio software is used for the calculation [18]. The PBE under the generalized gradient approximation (GGA) is chosen to deal with the electronic exchange-correlation energy problem between electrons [19], and the ultrasoft pseudopotential is used to describe the interactions between valence electrons and ions [20]. Considering the economy of calculation cost and the accuracy of calculation
results, the convergence of the interface model was tested by selecting the truncation energy of the reciprocal space as 300 eV, the K-point sampling integral of the Brillouin zone as $5 \times 4 \times 1$, and the convergence criteria: the total energy is less than $1.0 \times 10^{-5}$ eV/atom, the average atomic stress is less than 0.5 eV nm$^{-1}$, the tolerance offset is less than 0.02 nm, and the maximum stress deviation is less than 0.1 GPa. Firstly, the Ag and Ni cell structures were optimized using the BFGS algorithm \cite{21}, and the interfaces were constructed based on the optimized models. The Ag/Ni interfaces before and after doping were optimized using the above calculation parameters, and after obtaining a more stable state, the optimized systems were simulated and analyzed for substitution energy, separation work, interface energy, population, and density of states. The valence electron groupings considered in the calculations are: Ag 4d$^{10}$5s$^1$, Ni 3d$^8$4s$^2$, Co 3d$^7$4s$^2$, Mo 4p$^6$4d$^5$5s$^1$.

2. Simulation and analysis

2.1. Priority placement of doped elements

To study the preferential occupancy of doped elements at the Ag/Ni interface, the substitution energy of doped atoms at different positions is calculated in this paper \cite{22}. Substitution energy equation:

$$E_{\text{total}}^{\text{Ag}/\text{Ni} \rightarrow X} = (E_{\text{total}}^{\text{Ag}10/\text{Ni}7 \rightarrow X} + \mu_X) - (E_{\text{total}}^{\text{Ag}10/\text{Ni}8} + \mu_X)$$

In the formula: $E_{\text{total}}^{\text{Ag}/\text{Ni} \rightarrow X}$ indicates the substitution energy of the Ni atom at the interface when it is replaced by the dopant atom; $E_{\text{total}}^{\text{Ag}10/\text{Ni}7 \rightarrow X}$ indicates the total energy of the interfacial system after the substitution; $E_{\text{total}}^{\text{Ag}10/\text{Ni}8}$ indicates the total energy of the interfacial system before the substitution; $\mu_i$ ($i = \text{Ni}, X$) indicates the chemical potential of Ni or X.

The substitution energies of Co and Mo for a Ni atom with free relaxation are listed in Table 1. The substitution energies at positions 1 and 2 for Co doping of the Ag/Ni interface are negative, indicating that doping at this position is easy to carry out, while the substitution energy obtained from doping at position 3 is positive, i.e., the substitution at this position is relatively difficult; the substitution energy of Mo at position 3 is negative and relatively minimal. In summary, Co is preferentially occupied at position 1 and Mo is preferentially occupied at position 3. The subsequent analysis takes the preferential occupation of each element as the object of study.

2.2. Stability analysis

The source of cracks in AgNi contact material mainly comes from the interface between the Ag and Ni phases, and the raised tearing ribs with a large degree of plastic deformation form around the tough nest at the contact fracture \cite{23}, which is due to the weak bonding at the Ag/Ni interface. Impurity atoms are easily enriched at the interface, during the electrical contact, the arc acts preferentially at the interface of the substrate Ag, and the change in electronic behavior is only limited to a small area at the Ag/Ni interface. The newly generated structure at the interface has a direct impact on the overall performance of the composite material, so the stability analysis and electronic structure analysis at the interface are used to study the effect of doping on the anti-melt welding performance of AgNi contact material.

2.3. Interface bonding stability

Separation work and interfacial energy are introduced to analyze the stability of Ag/Ni interfacial bonding and the strength of interfacial bonding \cite{24}.

The work of separation ($W_{\text{sep}}$) refers to the energy required to separate the stable interface into two independent and infinitely distant free surfaces. The formula for calculating the work of separation ($W_{\text{sep}}$):
In the formula: $E_{\text{Ag}}^{\text{lab}}$ indicates the total energy of Ag free surface system; $E_{\text{Ni}}^{\text{lab}}$ indicates the total energy of Ni free surface system; $E_{\text{Ag},\text{Ni}}^{\text{int},\text{Ni}()}^{\text{relax}}$ indicates the total energy of Ag free surface system; $A$ indicates the interface area.

Interface energy ($\gamma_{\text{int}}$) represents the difference in energy per unit surface area caused by the formation of a complete interface between two free surfaces. The formula for calculating the interface energy:

$$\gamma_{\text{int}, \text{Ag}/\text{Ni}} = \sigma_{\text{Ag}} + \sigma_{\text{Ni}} - W_{\text{sep}, \text{Ag}/\text{Ni}}$$

In the formula: $\sigma_{\text{Ag}}$ indicates the surface energy of Ag free surface; $\sigma_{\text{Ni}}$ indicates the surface energy of Ni free surface; $W_{\text{sep}, \text{Ag}/\text{Ni}}$ indicates the separation work at the Ag/Ni interface.

The separation work and interface energy of Ag/Ni interface before and after Co and Mo doping are listed in Table 2. The Ag/Ni separation work of Co and Mo doping is 0.3931 J m$^{-2}$ and 0.4878 J m$^{-2}$ respectively, which is 91.1035% and 137.1415% higher than the separation work of the intrinsic Ag/Ni interface. The results indicate that more energy is required to separate the Ag/Ni interface after doping, so the doping of Co and Mo can make the Ag/Ni interface more stable. The Ag/Ni interface energy after doping is reduced to different degrees. The interface energy of Ag/Ni interface after doping with Mo element is 0.6138 J m$^{-2}$, which is the lowest value, and the Ag/Ni interface energy of doped Co is slightly improved, but it is still smaller than the undoped Ag/Ni interface energy. After doping, the energy required to construct the interface is reduced and the interface is easier to form.

The doping of Co and Mo significantly improved the bonding strength of Ag/Ni interface, strengthened the bonding force of Ag and Ni two-phase interface, and enhanced the stability of interfacial bonding, so the doping has a positive effect on improving the anti-melting weldability of AgNi contact material, among which the effect of Mo doping on the bonding strength of AgNi interface is the most obvious.

### 2.3.1. Thermodynamic stability

In order to analyze the thermodynamic stability of the Ag/Ni interface, the magnitude changes of enthalpy change values before and after Co and Mo doping were calculated in this paper (as in Table 2). The formula for the enthalpy change values [25]:

$$\Delta H = H_{\text{End}} - H_{\text{Ini}}$$

In the formula: $\Delta H$ indicates the enthalpy change value; $H_{\text{End}}$ indicates the energy of the product; $H_{\text{Ini}}$ indicates the energy of the reactants.

When the enthalpy change value is negative, it means that the products are thermodynamically stable, and the larger the absolute value, the more energy is released from the reaction and the more stable the products are. The enthalpy change of the system before and after doping is negative, and the absolute value of the enthalpy change of the Ag/Ni interface doped with Co and Mo elements increases in turn. Both of them are larger than the absolute value of the enthalpy change of the undoped system, and the doping improves the thermodynamic stability of the system, among which the most stable is the Mo-doped Ag/Ni interface model.

### 2.4. Electronic structure

#### 2.4.1. Population analysis

In order to analyze the electron gain and loss of each atom in the Ag/Ni interface before and after Co and Mo doping and the strength of bonding between atoms, the atom population and bond population between each atom before and after Ag/Ni interface doping were calculated in this paper (as shown in Tables 3 and 4), and the data in the tables were averaged.

From the analysis of the data in Table 3, the atom populations of Ag and Ni in the Ag/Ni interface are $-0.0213$ and $0.0275$, respectively, with Ag gaining electrons and carrying a negative charge and Ni losing electrons and carrying a positive charge. After the doping of the Ag/Ni interface, the atom populations of the doped Co and Mo are positive, and their values are much larger than those of Ag and Ni, and the loss of electrons of the doped atoms is strong. The electron transfer at the Ag/Ni interface is more obvious after doping, and the
bonding of atoms is more stable, which is beneficial to enhance the stability of interfacial bonding. Among them, Mo doping has the most drastic electron transfer and the most stable bonding at the Ag/Ni interface.

Compared with the undoped Ag/Ni interface, the doped interface increased the bonding of Ni-Co and Ni-Mo, and the number of bond population of Ni and doped atoms was higher than that of Ni and Ag. The bonding effect was obvious, which strengthened the bonding strength of Ag/Ni interface, among which the number of Ag-Ni bond population increased by 38.89% after Mo doping, which had the most obvious effect on the enhancement of Ag/Ni bonding strength. It is consistent with the results of stability analysis.

2.4.2. Analysis of state density
The state density can characterize the bonding between doped atoms and atoms at the Ag/Ni interface. It can be used to analyze the distribution of electrons at the interface. Figure 2 shows the Ag/Ni interface state density before and after doping Co and Mo.

Figure 2(a) shows the total state density and separate state density at the undoped Ag/Ni interface. The energy is mainly provided by the 5s and 4d states of Ag atom and the 4s and 3d states of Ni atom, and the energy is concentrated in the range of $-10 \sim 25$eV. In the range of $-5 \sim -3.3$eV, Ag(4d), Ni(3d) and a small amount of Ni(4s) are involved in the overlapping hybridization.

Figure 2(b) shows the Ag/Ni interfacial state density of Co doped. Co(3d) and Ni(3d) participate in hybridization within the energy range of $-3 \sim 0.3$eV, and a strong resonance wave peak appears near $-0.2$eV, indicating that there is a strong metal bond between Co and Ni. Figure 2(c) shows the Ag/Ni interfacial state density of doped Mo. There is a Bonding peak between Ni and Mo at $-4.8 \sim 0.3$eV, which mainly depends on the hybridization of Mo(4d), Mo(4p) and Ni(3d) electron orbitals.

The main reasons for the improvement of interface stability are the enhancement of Ag-Ni metal bond bonding strength and the enhancement of orbital hybridization. The doping of Co and Mo not only increases the orbital hybridization between doped atoms and Ni, but also increases the hybridization of s and d orbitals of Ag and s and d orbitals of Ni, thus improving the bonding strength of Ag-Ni and the bonding stability of Ag/Ni interface.

3. Experimental and analysis

3.1. Preparation of AgNi alloy contact material by powder metallurgy method
AgNi contact samples were prepared using commercially available Ag powder, Ni powder, Co powder, Mo powder and ethanol. This test corresponds to the simulation. According to the mass ratio of Ag powder and Ni powder 70:30, 10 g AgNi powder including 7g Ag powder and 3g Ni powder is configured. The AgNi contact material doped with Co and Mo is weighed according to the atomic ratio conversion in the simulation (as shown in table 5). The ground powder was dried at 120 °C for 1 h, and high-energy ball milling and mixing was carried out by an omni-directional planetary ball mill for 2h, so that the Ag, Ni and doped powders were evenly mixed.

Diffraction phase analysis of AgNi alloy powder samples before and after doping shows that doping is not found in the alloy powder with Co and Mo doping, but the diffraction peak of Ni widens, indicating that the doping is solidly dissolved in the matrix. XRD verifies that the substituted doping interface model established by

| Table 3. Atom populations at Ag/Ni interface. |
|--------------|---------|------|------|------|
| Model        | Ag      | Ni   | Co   | Mo   |
| Ag/Ni        | -0.0213 | 0.0275| -    | -    |
| Ag/Ni+Co     | 0.0100  | -0.0255| 0.1400| -    |
| Ag/Ni+Mo     | -0.0269 | -0.1555| -    | 0.2130|

| Table 4. Bond populations at Ag/Ni interface. |
|--------------|---------|------|------|
| Model        | Bond population |
|              | Ag-Ni   | Ni-Co | Ni-Mo |
| Ag/Ni        | 0.1800  | -     | -     |
| Ag/Ni+Co     | 0.1843  | 0.1940| -     |
| Ag/Ni+Mo     | 0.2500  | -     | 0.4883|
Figure 2. density of states.

Table 5. Mass ratio of Ni powder with Co- and Mo-doped.

| Reagent | Atomic ratio | Mass ratio |
|---------|--------------|------------|
| Ni: Co  | 91.6354:8.3646 | 2.7491:0.2509 |
| Ni: Mo  | 87.0619:12.9381 | 2.6118:0.3882 |
The simulation model corresponds to the powder metallurgy method in the experiment, which indicates that the theoretical simulation model established in this paper matches the experiment.

The fully mixed AgNi composite powder was put into the mould of the tablet press for pressing and forming. The initial pressure was 10 MPa (17.6 tf), and the pressure was held for 10 min to make a cylinder with a diameter of 20 mm and a thickness of 3.5 mm. The cylinder was sintered at 700 °C for 4 h in a vacuum tube furnace and held for 90 min. After that, repressing (repressing pressure 15 MPa (26.4 tf), holding for 10 min), refiring (refiring temperature 650 °C, sintering 4 h, holding for 60 min), and tripressing (tripressing pressure 20 MPa (35.2 tf), holding for 10 min) were carried out. Finally, the sample was polished and cut to obtain a diameter of 3.2 mm.

3.2. Wettability analysis

With the increase of interfacial bonding strength, interfacial bonding energy and interfacial bonding stability, the interfacial wettability is improved [26]. Therefore, the simulation conclusion is verified by the test of wetting angle. The wetting angle between Ni substrate and Ag before and after doping was measured by the seat drop method (figure 3), and the influence of doping on the interface characteristics of Ag/Ni was analyzed [27].

In order to intuitively characterize the improvement effect of doping on the wettability of Ni and Ag, the average wetting angles between Ni substrate and Ag before and after Co and Mo doping were counted (in table 6). The average wetting angle between undoped Ni and Ag is 88.8500°, which is much larger than the average wetting angle between doped Ni and Ag, indicating that doping has a positive effect on improving the wetting angle between Ni and Ag. After the addition of trace dopants Co and Mo to Ni, the surface tension angle of the Ag/Ni interface decreases, and the adhesion is enhanced. The interface between Ag and Ni is more firmly bonded, which improves the wettability of Ag on the contact surface. The average wetting angle between Ni doped with Mo and Ag is the lowest, which is 50.9285% lower than that between Ni and Ag without doping. The improvement effect on the wettability between Ni and Ag is the most obvious, which verifies the conclusion that the simulation analysis above is beneficial to improve the interfacial bonding stability after doping. The doping enhances the spread of liquid Ag on the contact surface, reduces the splash loss of the material, inhibits the arc.

Figure 3. Wetting angle test.
ablation of the contact, and further improves the anti-welding performance and anti-arc erosion of AgNi contact material.

3.3. Electrical contact experiments.
Anodic transfer is the main form of material transfer [28], and the selection of contact material with excellent performance as the anode will have a good effect on improving the electrical life of the material. Therefore, Co and Mo doped AgNi contact material is selected as the asymmetric pairing of the anode to conduct the electric contact experimental study.

3.3.1. Analysis of fusion weldability
In view of the contact materials after polishing, the electrical contact performance of the contact samples was measured by the electrical contact material testing system (JF04D). The system protection voltage ± 60 V, DC voltage 24 V, DC current 15 A, closing pressure 86 cN, on-off times 25000 were adopted in the test. The arc energy, arc time and welding force were measured. The electronic balance (JA3003N) was used to measure the amount of contact material transfer before and after the electrical contact test.

The electric contact performance parameters, such as arc energy, arc time, average welding force and maximum welding force, were obtained by electric contact test (in table 7). A simple analysis shows that the doping of Co and Mo has a positive effect on the electrical contact properties of AgNi contact materials. The average fusion welding power and the maximum fusion welding power of the AgNi contact materials doped with Co and Mo decreased, and the fusion welding power of the contact materials doped with Mo decreased obviously, because Mo and Ni could form brittle intermetallic compounds, furthermore, the Brittleness of the AgNi material is enhanced, and the fusion welding force is reduced. Moreover, the chemical affinity of Mo and the Substrate Ag is small, which can further reduce the fusion welding force of the metal after being welded together.

3.3.2. Analysis of resistance to arc erosion
High temperature arc is generated in the on-off process of electrical contact. A large amount of Joule heat is generated by arc combustion, and the temperature rises to the melting point of Ag matrix of the contact, resulting in metal splashing and loss, ablation of electrical contact material and shortening of electrical life.

According to the data analysis in table 7, compared with undoped AgNi contacts, the arc burning energy and arc burning time of AgNi contacts doped with Co and Mo are reduced to varying degrees, indicating that the doping of the above two elements have a positive effect on improving the arc erosion resistance of AgNi. Among them, Mo-doped AgNi as the anode of asymmetric contact pair, its arc energy and arc time improved greatly. The reason is that the stability of the contact material is improved, and the AgNi is kept suspended in the molten metal pool under the action of arc, which inhibits AgNi agglomeration on the contact surface and improves the uniformity of structure and composition. When the arc is extinguished, the molten metal pool solidifies, and Mo and Ni precipitate and distribute evenly in the matrix, which plays a role of dispersion strengthening, ensuring that the electrical contact property of the contact material will not deteriorate, and enhancing its arc erosion resistance.

| Table 6. Wetting angles. |
|-------------------------|
| Sample     | Average wetting angle/° |
| AgNi       | 88.8500                  |
| AgNiCo     | 79.5000                  |
| AgNiMo     | 43.6000                  |

| Table 7. Electrical contact performance. |
|----------------------------------------|
| Contact materials | Arc energy /mJ | Arc duration /ms | Welding force /cN | Maximum welding force /cN |
|-------------------|----------------|------------------|-------------------|---------------------------|
| AgNi-AgNi         | 176.1688       | 8.7276           | 62.8581           | 303.1023                  |
| AgNi-AgNiCo       | 169.4741       | 8.6950           | 56.1342           | 224.0206                  |
| AgNi-AgNiMo       | 157.5354       | 8.6809           | 45.3084           | 97.0581                   |

Mater. Res. Express 9 (2022) 086301 J Wang et al
### 3.3.3. Measurement and analysis of material loss

After 25000 times of electrical contact experiment, the cathode and anode electrical contacts have different degrees of fusion welding and erosion, leading to the material transfer of cathode and anode contact. The smaller the material transfer amount, the better the thermal stability of contact material, the better the fusion welding resistance of AgNi contact material.

Table 8 lists the change of cathode and anode contact material quality and the quality of the contact. The data in the table shows that anodic transfer is the main form of material transfer, Co, Mo doping can reduce cathode and anode contact quality changes, one of doped Mo AgNi contact quality loss is far less than that without doping AgNi contact. This is because the doping of Mo makes the Ag-Ni metal bond stronger, which is conducive to the densification of the material sintering, thus reducing the material transfer at the poles of the contact. The material loss changes analyzed here are consistent with the above analysis results.

### 4. Conclusion

In this paper, based on the first principles, the influence of metal Co and Mo doping on the Interface properties of Ag/Ni was studied. The AgNi contact material was prepared by powder metallurgy method, and its electrical contact properties were studied to verify the correctness of the simulation results.

1) Doping Co and Mo facilitates Ag/Ni interfacial bonding and strengthens interatomic bonding and orbital hybridization. The Ag/Ni interfacial doping results in more obvious charge transfer and more stable bonding. The average Ag-Ni bond population increases, the interaction between Ag and Ni at the interface is enhanced, and the interface bonding stability is improved.

2) After doping, the spreading degree of molten Ag on the doped Ni substrate is improved, and the wettability between Ni and Ag is improved, so that Ni is more easily dispersed into the Ag molten pool under the action of arc. The viscosity of molten pool is enhanced, the splash loss is reduced, and the electrical contact performance of contact material is improved.

3) Co and Mo doping can shorten the arc burning time and arc burning energy of AgNi contacts, alleviate the ablative degree of contacts, and enhance the arc erosion resistance of contact materials. The average fusion welding force is reduced, and the probability of fusion welding occurs is small, which has a positive impact on the improvement of the fusion welding resistance of contact materials. Among them, Mo doping has the best effect on the improvement of fusion welding resistance and arc erosion resistance of AgNi contacts, which is consistent with the simulation results.

In summary, the above analysis proves that Co and Mo doping has a positive effect on improving the properties of AgNi contact materials, among which Mo doping has the most obvious improvement effect. Moreover, the simulation analysis results are verified by experiments, which confirms the feasibility of first-principle analysis and provides guidance for subsequent experimental research on AgNi electrical contact materials.

### Acknowledgments

Thanks to all authors for their contributions to this article: JW designed the experiments and provided the materials and equipment needed for the experiment; JJ and DC carried out the experiments; PG and NL assisted with the experiments; JW and JJ analysed simulation results and experimental results; and JJ wrote the manuscript.
Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Funding

This study was funded by Central Leading Local Science and Technology Development Fund Project (216Z1011G) and National Natural Science Foundation of China (51777057).

ORCID iDs

Jiying Jia \(\text{https://orcid.org/0000-0001-8766-1706}\)

References

[1] Wang J, Li D and Wang Y 2014 Journal of Alloys & Compounds 582 1–5
[2] Wang Q X 2021 Journal of SolidState Electrochemistry 1 1–9
[3] Wang H and Yuan H 2017 IEEE Holm Conference on Electrical Contacts 17 221–4
[4] Hao X, Wang X H and Zhou S M 2018 Mater. Chem. Phys. 215 327–33
[5] Fan Y, Huang X W and Wang Y X 2013 Electrical material 02 3–7
[6] Han J F 2018 Thesis Work
[7] Yang C L, Zhang X F and Yan X F 2021 Journal of SolidState Electrochemistry 11 1–9
[8] Geng X L, Yang R and Liu J L 2020 Electroplating and finishing 39 255–9
[9] Zhu M H 2021 Thesis Work
[10] Chen J, Yin Z L and Zhang H Z 2019 Nonferrous Metals Engineering 9 1–6
[11] Li Z B, Cheng L C and Zou J Y 1995 Electrical alloy 02 20–2
[12] Dao T Y R and Shi G Z 1999 Japan: CN1047460C
[13] Zhang Y, Wang J Q and Kang H I 2021 Journal of Electrical Engineering Technology 36 1587–95
[14] Guo T F, Fu C and Wang J B 2015 Electrical material 02 34–8
[15] Guan W M, Pan Y and Zhang K H 2010 Rare Met. Mater. Eng. 39 1339–43
[16] Gai Y B, Tang F W and Hou C 2020 Journal of Metal Science 56 1036–46
[17] Ran X J and Zhou Land Huang F X 2022 Atomic and Molecular physics 39 136–44
[18] Peng Y, Zhou D W and Xu S H 2012 Rare Met. Mater. Eng. 41 302–6
[19] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[20] David V 1990 Physical Review B 50th Anniversary Milestones 41 7892
[21] Zhu C Y, Byrd R H and Lu P H 1997 ACM Trans. Math. Softw. 23 550–60
[22] Xiong H H, Liu Z and Zhang H H 2017 Journal of physics 66 287–93
[23] Shi P and Xiong E T 2011 Material for mechanical engineering 35 73–5
[24] Xu P Y, Wang Y F and Gao H Y 2018 Journal of the Non-ferrous metal 28 39–45
[25] Xu J T, Wang J Q and Zhu Y C 2022 J. Compos. Mater. 01 1–13
[26] Wu Y, Long F and Shen F Y 2009 Rare Met. Mater. Eng. 38 525–8
[27] Wang J Q, Chang Y Q and Zhu Y C 2021 Mater. Res. Express 8 066528
[28] Li H and Hou Y B 2005 Electric Material 03 12–4