Investigating Properties of Electrodeposited Ni-W Alloy Using Empirical Electron Theory of Solids and Molecules

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Abstract. To study deposited Ni-W alloy on electronic level, empirical electron theory of solids and molecules (EET) was used to calculate valence electron structures (VES). In addition, high-resolution transmission electron microscope (TEM) was used to identify crystal features. Regular arrangement exists according to concentric rings diffraction pattern. That provides an experimental basis for crystal VES. And VES of Ni-W alloy was contrasted to pure Ni metal. It is indicate that melting point, strength, corrosion resistance, and wear resistance of Ni-W alloy are significantly higher than those of pure Ni metal

Introduction

Melting point, strength, corrosion resistance, and wear resistance data of electrodeposited Ni-W alloy layer are shown in Table1 [1]. Ni-W alloy layer is suitable for bearings, pistons, and cylinders in corrosive environment and wear conditions, as well as for certain products in the petroleum industry requiring surface coating [2]. Zhou studied 10 kind temperature and PH value effect on the coating structure [3]. Based on hemispherical nuclei, diffusion control point instantaneous nucleation, and consecutive crystallization nucleation mechanism of dimensionless equation, Li studied nucleation mechanism of Ni-W alloy under point crystallization electric nucleation [4]. In addition, Yang studied the plating process effect on internal stress [5]. However, no study has report composite sedimentary characteristics on electronic structure level.

Table 1 Hardness, wear, and corrosion resistance of 3 metals.

Plating metal	Micro-hardness after heat treatment [HV]			Grinding weight loss [mg]	Erosion time [h]	
	200˚C	400˚C	600˚C		15%HCL	1 mol/L HNO_3
Cr	780	736	242	23.8	1	0.6 Completely
Ni	—	—	—	—	0.3	0.1 Completely
Ni-W(44%)	682	1210	631	1.3	72	24 Partly

Valence electron structure (VES) features were studied by empirical electron theory of solids and molecules (EET). In addition, the bond length different (BLD) method is a theoretical basis from cell structure to VES. VES values of deposited Ni-W were calculated and contrasted to pure Ni.

Experimental and theoretical basis

Experimental basis. Fig. 1 shows high resolution transmission electron morphology electrodeposited Ni-W alloy (atom ratio 3:1). Due to plating bath composition, current density and other process factors, Ni-W alloy has partly irregular atomic arrangement. However, regular

arrangement also exists according to concentric rings diffraction pattern. That provide experimental basis for electrodeposited Ni-W alloy VES calculated.

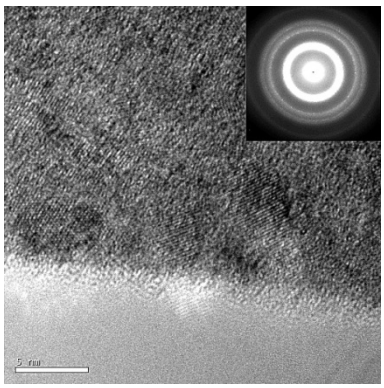

Fig. 1. High resolution transmission electron morphology of electrodeposited Ni-W alloy.

Theory basis. The BLD method is used to calculate the valence electron structure of solid and molecule. It is to solve atom state and covalent bond in specified solid and molecule. So the premise is to know crystal type, lattice parameters and atomic coordinates [6].

The covalent bond formula in EET is given by

$$D_{na}^{u-v} = R_u(1) + R_v(1) - \beta \lg n_a \quad (1)$$

where u, v are the two atoms forming bond; α is bond ordinal; $R_u(1)$ and $R_v(1)$ are atom radius of hybrid state, respectively; n_α is covalent electron pairs number; and β is coefficient.

According hypothesis that theory bond distance difference is equal to experiment bond distance difference, researchers can obtain the theory distance D_{na}^{u-v} by solving n_a equation set. Bond distance difference, $\Delta D/nm = \left|D_{n\alpha}/nm - \overline{D}_{n\alpha}/nm\right| \leq 0.005\ nm$, is the criterion to determine atom hybrid state in given system. Where $D_{n\alpha}/nm$ is experimental bond distance; $\overline{D}_{n\alpha}/nm$ is theoretical bond distance.

Hybrid tables of Ni and W atoms. When calculating hybrid table, specific parameters Ni cell are defined as follows:

Lattice type: A1, fcc, Fm3m (No.225);

Equivalent point location: (0, 0, 0; 1/2, 1/2, 0);

Lattice atoms: A = 4.

The specific parameters of W cell are as follows:

Lattice Type: A2, bcc, Im3m (No.229);

Equivalent point location: (0, 0, 0; 1/2, 1/2, 1/2);
Lattice atoms: A = 2.

Hybrid of Ni and W atoms are shown in Tables 2 and 3 respectively. As can be seen, σ is miscellaneous order number; C_h is head state content; C_t is end state content; n_t is total valence electrons number; n_l is lattice electrons number; n_c is covalent electrons number; R (1) / nm is single bond half distance.

Table 2 Hybrid state parameters of Ni cell.

σ	C_h	C_t	n_t	n_l	n_c	R(1)[nm]
1	1.0000	0	6.0000	1.0000	5.0000	0.1195
2	0.9987	0.0013	6.0025	0.9987	5.0038	0.1195
3	0.9987	0.0013	6.0025	0.9987	5.0038	0.1195
4	0.9923	0.0077	6.0153	0.9923	5.0230	0.1194
5	0.9539	0.0461	6.0922	0.9539	5.1383	0.1190
6	0.9539	0.0461	6.0922	0.9539	5.1383	0.1190
7	0.9370	0.0630	6.1259	0.9370	5.1889	0.1189
8	0.8070	0.1930	6.3861	0.8070	5.5791	0.1176
9	0.7734	0.2266	6.4532	0.7734	5.6798	0.1172
10	0.7093	0.2907	6.5815	0.7093	5.8722	0.1166
11	0.6847	0.3153	6.6306	0.6847	5.9459	0.1163
12	0.5589	0.4411	6.8821	0.5589	6.3232	0.1151
13	0.2816	0.7184	7.4368	0.2816	7.1552	0.1123
14	0.0992	0.9008	7.8017	0.0992	7.7025	0.1105
15	0.0640	0.9396	7.8793	0.0640	7.8189	0.1101
16	0.0541	0.9459	7.8918	0.0541	7.8377	0.1100
17	0.0323	0.9677	7.9354	0.0323	7.9031	0.1098
18	0	1.0000	8.0000	0	8.0000	0.1095

Table 3 Hybrid state parameters of W cell.

σ	C_h	C_t	n_t	n_l	n_c	R(1)[nm]
1	1.0000	0	6.0000	2.0000	4	0.1385
2	0.8239	0.1761	5.6479	1.6479	4	0.1322
3	0.8239	0.1761	5.6479	1.6479	4	0.1322
4	0.8239	0.1761	5.6479	1.6479	4	0.1322
5	0.6904	0.3096	5.3807	1.3807	4	0.1274
6	0.6193	0.3807	5.2386	1.2386	4	0.1249
7	0.5131	0.4869	5.0261	1.0261	4	0.1211
8	0.3728	0.6272	4.7456	0.7456	4	0.1161
9	0.3728	0.6272	4.7456	0.7456	4	0.1161
10	0.3728	0.6272	4.5361	0.5361	4	0.1161
11	0.3728	0.7319	4.5361	0.5361	4	0.1124
12	0.2681	0.7319	4.4414	0.4414	4	0.1124
13	0.2207	0.7793	4.3425	0.3425	4	0.1107
14	0.1712	0.8288	4.3425	0.3425	4	0.1089
15	0.1180	0.8820	4.2361	0.2361	4	0.1070
16	0.0445	0.9555	4.0889	0.0889	4	0.1044
17	0.0445	0.9555	4.0889	0.0889	4	0.1044
18	0	1.0000	4.0000	0.0000	4	0.1028

Results and discussion

VES of Ni and Ni-W alloy. Lattice parameter of Ni cell is 0.3524 nm at room temperature. Experimental bonds that can not be ignored were scanned separately with 18 hybrid levels in Table 2. Tool software is MATLAB. 3 hybrid levels meet solution conditions, $\Delta D/nm = \left|D_{nu}/nm - \overline{D}_{nu}/nm\right| \leq 0.005\ nm$. The smallest ΔD exists level 12. The VES is shown in Table 4. I_a is equal bond number.

Table 4 Valence electron structure of Ni cell.

Bond	Bonded atom	I_a	n_a	△D[nm]
A	Ni-Ni	12	0.5210	0.0020
B	Ni-Ni	6	0.0099	0.0020
C	Ni-Ni	24	0.0005	0.0020

Due to W atom 9.6% radius difference contrast Ni, substitutional solid solution can be formed. The model [7] is shown in Fig. 2. A couple Ni atoms are substituted by W in two opposite surface center positions. In EET, Ni atoms at surface center are different from vertexes. That means they can on different hybrid states, so 3 kind atoms in a cell.

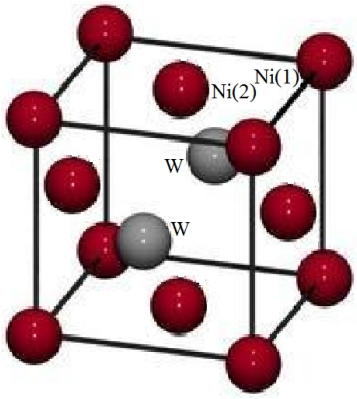

Fig. 2. Diagram of the Ni-W alloy cell.

Experimental bonds that can not be ignored were scanned separately with 18 hybrid levels in table 2 and 3. 1952 hybrid state combination meet solution conditions. Hence, the equivalent hybrid number were $\sigma_N^{'} = \sqrt[5]{1952} \approx 12$. The combination has the smallest ΔD determines VES, as shown in Table 5.

Table 5 Valence electron structure of Ni-W alloy cell.

Bond	Bonded atom	I_a	n_a	△D[nm]
A	Ni(2)-Ni(2)	2	0.6756	8.7545×10^{-5}
B	Ni(1)-Ni(2)	4	0.4605	8.7545×10^{-5}
C	Ni(2)-W	4	0.4185	8.7545×10^{-5}
D	Ni(1)-W	2	0.2853	8.7545×10^{-5}
E	Ni(1)- Ni(2)	1.5	0.0060	8.7545×10^{-5}
F	W-W	1.5	0.0049	8.7545×10^{-5}
G	Ni(2)- Ni(2)	3	0.0129	8.7545×10^{-5}
H	Ni(1)- Ni(2)	8	0.0004	8.7545×10^{-5}
I	Ni(1)-W	4	0.0003	8.7545×10^{-5}
J	Ni(2)-W	12	0.0004	8.7545×10^{-5}

Discussion.The larger n_A, the stronger the structure, which means higher melting point when heated, higher strength when pressed or pulled [8,9]. For Ni-W alloy, n_A (0.6756) increased 29.7% to pure Ni metal (0.5210), as shown in Tables 4 and 5. Therefore, the Ni-W alloy has higher melting point, higher strength, higher corrosion resistance.

Meanwhile, the greater σ_N, the greater the stability. A hybrid steady state is damaged by corrosion, wear, a new steady state will be formed promptly. Equivalent configuration (12) is 4 times to pure Ni, so Ni-W alloy has higher corrosion and higher wear resistance.

Conclusion

1) Concentric rings diffraction determines electrodeposited Ni-W alloy crystal characteristics.

2) n_A increased 29.7%, and σ_N increased 3 times. Thus, Ni-W alloy has higher melting point, higher strength, higher corrosion resistance and higher wear resistance.

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