EFFECT OF ALLOYING ON ELECTRONIC STRUCTURE, STRENGTH AND DUCTILITY CHARACTERISTICS OF NICKEL ALUMINIDE

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Aim of investigation — increasing of NiAl room temperature ductility by alloying with Fe, Cr, Co, Mo, B, La

Experimental techniques and conditions

Samples: Stoichiometric polycrystalline NiAl with addition of third element (Fe, Cr, Mo, Co) of 2.0 % at. , and B, La of 0.1 % at.
Processing: The alloys were produced with joint CaH_2 – reduction of the oxides mixtures (at 1175 °C, exposition time 8 hours). The produced powders were compacted by hydrostatic pressing (P = 500 MPa) and sintering at 900-1400 °C during six hours. Hot extrusion of the sintered rods 80 mm in diameter and 120 mm long was carried out at 850-1200 °C with drawing factor λ of approximately 3247. Rods with a diameter of 10-12 mm were produced.
Mechanical tests: Tensile tests; The compression test at the room temperature is the softest type of stress state of the metal.
Fractography: Fractography investigations were carried out using SEM JEOL JSM-U3.
Electron spectroscopy: The plasmon losses and valence band were investigated with electron spectroscopy. The experiments were performed in an UHV multitechnique system (VG ESCALAB MK2). The base pressure during these experiments was 10^{-10} Torr in the analyzer and preparation chambers. The electron gun EMU50 is used as excitation source. Monochromatized electron beam has the energy of 30.0eV. The backscattered electron peak has the FWHM = 28 meV. The spectra were recorded and accumulated in CAE mode at 2.0 eV pass energy. Each sample was cleaned by Ar^+ ion sputtering and annealing at 723 K under vacuum $1x10^{-10}$ Torr. After this treatment no traces of contamination were detected within AES and SIMS sensitivity.

Results

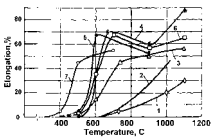
Mechanical properties

Alloying effects on the strength and ductility characteristics of nickel aluminide (compression test at room temperature). The alloyed specimens in compression test showed sufficiently high low-temperature ductility.

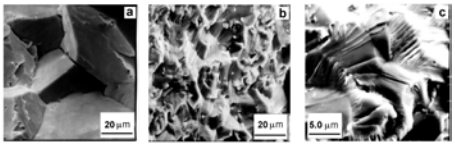
Fractography

Systematic investigation of the microrelief of fracture surfaces by SEM showed transformation of micromechanism of brittle fracture from inter-granular to quasi-cleavage with alloying of NiAl. Alloying of NiAl with Fe or Co increases the energy capacity of fracture and the occurrence of microplastic deformation. Alloying of nickel aluminide with B or La relieve transmission of dislocation slip across grain boundaries.

Alloy	$\sigma_{0.2}$, MPa	ε, %	ψ, %	Change of n_{eff}[1], %	Shift of Fermi level[2], ΔE_F, eV	Grain size, μm	Intergranular fracture, %	Microhardness Hμ, kg/mm²	Transition temperature, °C
NiAl	292	12.0	0	0	0	21	70	379.3	700
NiAl + 0.1% B	400	25.6	0	0	+0.2	7	5	384.1	430
NiAl + 0.1% La	311	29.5	70.0	0	-0.2	6	3	379.3	400
NiAl + 2% Fe	396	28.0	65.0	+1.23	-0.5	7	50	350.3	500
NiAl + 2% Co	384	30.8	69.0	+0.28	-1.0	9	45	327.0	450
NiAl + 2% Cr	421	24.8	60.8						
NiAl + 2% Mo	340	26.0	17.0	+0.2	+0.5	10	60	398.2	650

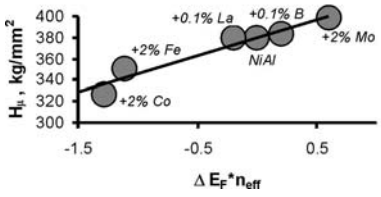


Elongation of NiAl alloys under testing at 400 1200 °C: 1 casted NiAl; 2 extruded NiAl; 3 NiAl(Mo); 4 NiAl(W); 5 NiAl(Fe); 6 NiAl(Cr); 7 NiAl(Co, B, La).



SEM images of inter-granular fracture of NiAl intermetallic (a), quasi-cleavage fracture of NiAl(Co) alloy(b) and dislocation slip transmission across grain boundaries in NiAl (La) alloy (c).

The shift of the Fermi level (ΔE_F) and variation of density of conduction electrons $-n_{eff}$ were found in doped NiAl. The results show good correlation between $E_F \cdot n_{eff}$ and micro-hardness of alloyed NiAl intermetallic.



Correlation between micro-hardness and electronic structure characteristics of alloys on base of NiAl.

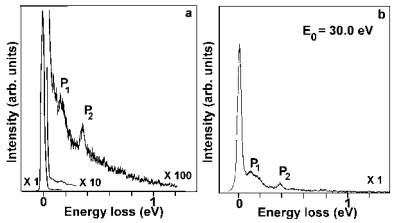
Adds of Mo, Fe, Co increase in this raw the fraction of metallic bond in the intermetallic lattice changing the electrons concentration on the Fermi level and moving it. With decrease of the covalent component of interatomic bonds the Peierls energy U_P and corresponding, Peierls barrier of plastic deformation σ_P:

$$\sigma = \frac{\pi}{\quad}$$, where a – lattice parameter; b – Burgers vector.

The dropping of σ_P increases plasticity and decreases strength of alloy. This effect is confirmed by good correlation between micro-hardness and electronic structure characteristics of alloys on base of NiAl.

Electronic structure

Alloying elements in NiAl intermetallic alter locally the electronic structure and bonding characteristics determining the fracture behavior and the dislocation mobility. We used as basic characteristics of electronic structure the concentration of conduction electrons n_{eff} measured from plasmon losses spectra and shift of the Fermi level ΔE_F comparing to pure NiAl.
Metallic component of interatomic bonds in NiAl increases at alloying by Cr, Fe, Co that leads to increase of the alloy plasticity.

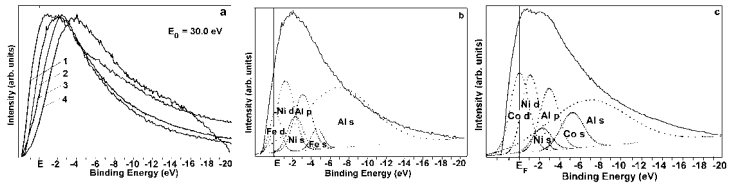


HREEL spectra of polycrystalline surfaces of NiAl (a) and NiAl(Fe) alloy (b). Primary beam energy 30 eV.

The plasmon peak intensity in the spectrum of primary electrons energy loss is connected with the excitation of collective oscillations among conduction electrons and determined by their concentration. This permits us to determine the effective concentration of conduction electrons on the basis of principles of dielectric theory of energy losses, using the integral intensity of plasmon peaks (I_m):

$$= \frac{\varepsilon}{\pi\hbar} \int \quad - -$$
$$\varepsilon$$

After normalizing an integral intensity for P_2 peaks to the respective intensities of backscattered electron lines, we could determine a change in effective density of conduction electrons in stoichiometric NiAl and alloys on base NiAl. Assuming that the concentration of conduction electrons n_{eff} is equal 1% in NiAl, we have estimated the relative change of n_{eff} in alloys.



Electron spectra in valence band region of alloys on base of nickel aluminide.(a): 1 NiA(Co) 2 NiAl(Fe); 3 NiAl; 4 NiAl(Mo); and interpretation of density-of-states in VB of alloyed intermetallic: (b) NiAl(Fe); (c) NiAl(Co).(E_0=30.0 eV).

For NiAl, the d-bonding states are occupied, E_F is located near the antibonding area of the total density-of-states, and the density-of –states at Fermi level - $N(E_F)$ is the relatively low. Alloying of NiAl by Fe Co and Mo significantly influence on the density-of-states in VB of intermetallic. The basis of chemical bonding for NiAl is the strong Ni–Al interaction caused by the hybridization of Ni d, s- and Al p-orbitals. Alloying NiAl by Fe or Co lead to a shift of E_F to the low energy region and to a substantial increase of $N(E_F)$: Fe and Co atoms cause an increase of Ni d-states (Figs b, c) and the largest contribution to $N(E_F)$. These results is good correlated with increasing plasmon losses in NiAl alloying by Fe, Co. For NiAl, when the Fe or Co additions (Me) occupy Ni sites, both the d – d bonding between Me and Ni atoms and Me – Al bonding increase in comparison to Ni – Ni and Ni – Al bonds in the lattice of intermetallic. By contrast, molybdenum adds lead to a shift of E_F to the high energy area and there is not large increase of $N(E_F)$.
The changes in the electronic structure due to the substitual atoms strongly depend on which sublattice the impurity occupies.
Obviously, site preference for Mo substitution must be the Al sublattice of intermetallic. For Fe and Co additions in NiAl, impurity atoms substituted at the Ni sublattice in stoichiometric NiAl.

Conclusions

Alloying with Fe, Cr, Co, Mo, B, La has a beneficial effect on the micro-mechanism of fracture and ductile-brittle transition temperature of alloys on base of NiAl. Volume fraction of intergranular failure is decreased from 70 % (for NiAl) to 5 % (for NiAl alloyed by 0.1%B). The energy of Fermi level E_F, concentration of electrons in conduction band n_{eff} and density of electron states near it $N(E_F)$ were changed in ternary alloys on base of NiAl. Correlation between the micro-hardness and $E_F n_{eff}$ was found.
According to theoretical consideration, these changes of electron structure of alloys can essentially alter the Peierls energy and the Peierls stress, decreasing the covalent component of interatomic bonds and increasing its metallic component. Improvement of the alloys plasticity is tied with above mentioned effects.

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