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Exploration of an electron work function – based strategy for tailoring materials

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Outline

1. **Background and electron work function (EWF)**

2. **Correlation between EWF and properties of materials**

3. **Can EWF be a design parameter for materials?**

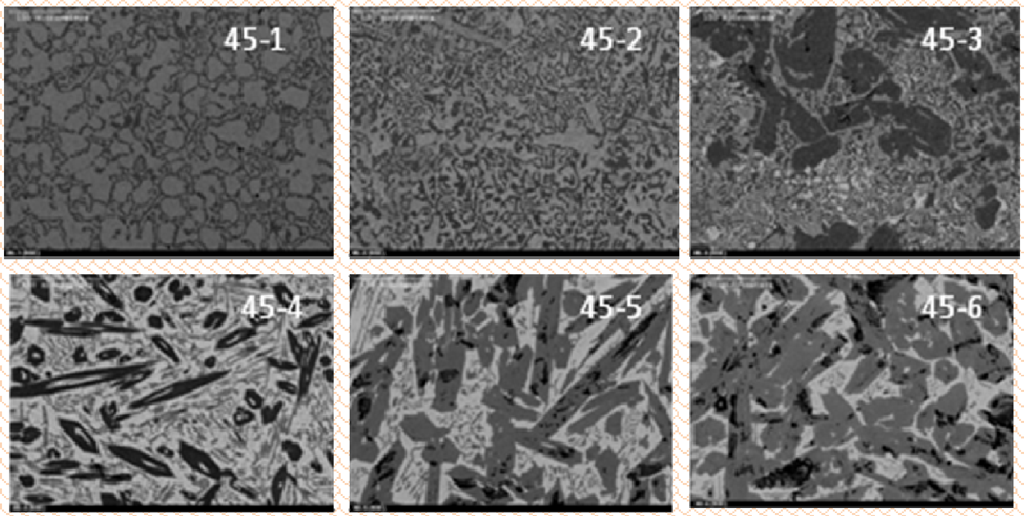
   - EWF and properties of Cu-Ni alloys

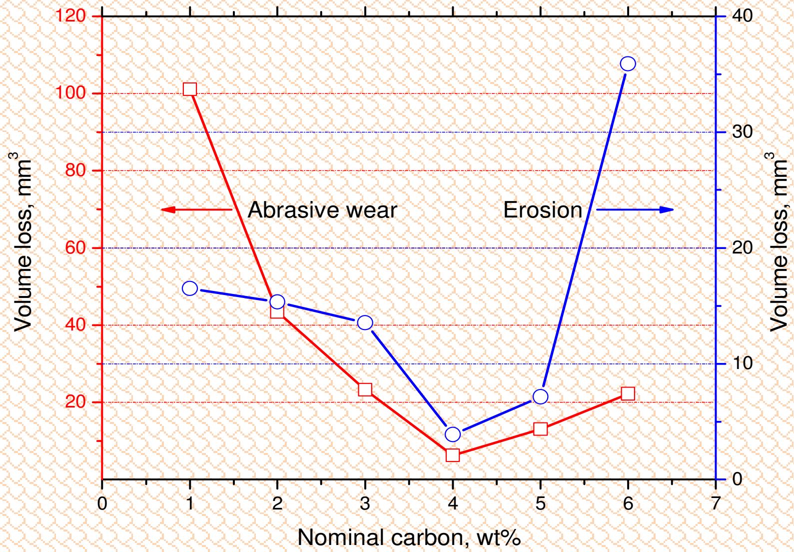
   - EWF and properties of multi-phases alloys

4. **Conclusions**

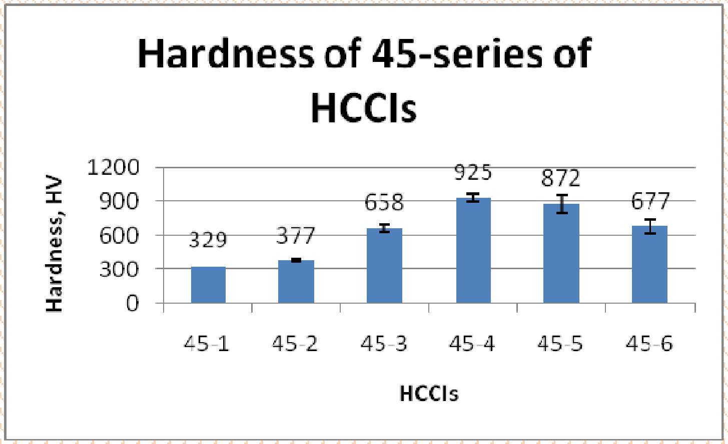
1. Background and electron work function (EWF)

Example: High-Cr cast iron - Increasing the volume fraction of carbides raises its hardness and resistance to wear. However, too many carbides deteriorate the material.

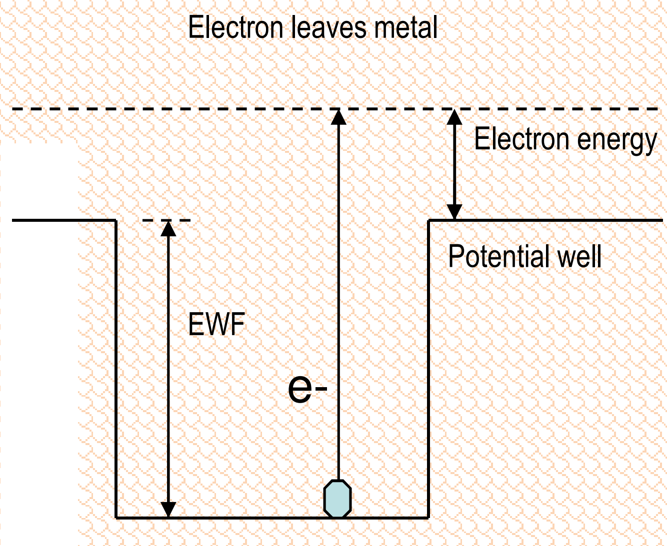




For multiphase alloys, strengthening the matrix without reducing the number of slip systems by appropriate solutes helps raise hardness while maintaining desired toughness.



In addition to the solubility and the difference in atomic size between solute and solvent, the inter-atomic interaction or atomic bonding is an important parameter for the effectiveness of solute-strengthening.



$$\varphi \propto n_s \quad \text{(Free electron density)}$$

Selection of elements based on electron work function (φ).

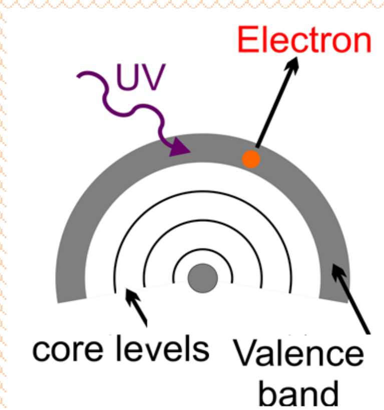
The work function is the minimum energy needed to move an electron at the Fermi level from inside a solid to its surface with zero kinetic energy

EWF is a fundamental parameter directly related to atomic bond strength, which determines many properties of materials.

EWF measurements

Methods: Employ electron emission from the sample induced by photon absorption (photoemission), by high temperature (thermionic emission), and by an electric field (field electron emission).

Ultraviolet photoelectron spectroscopy

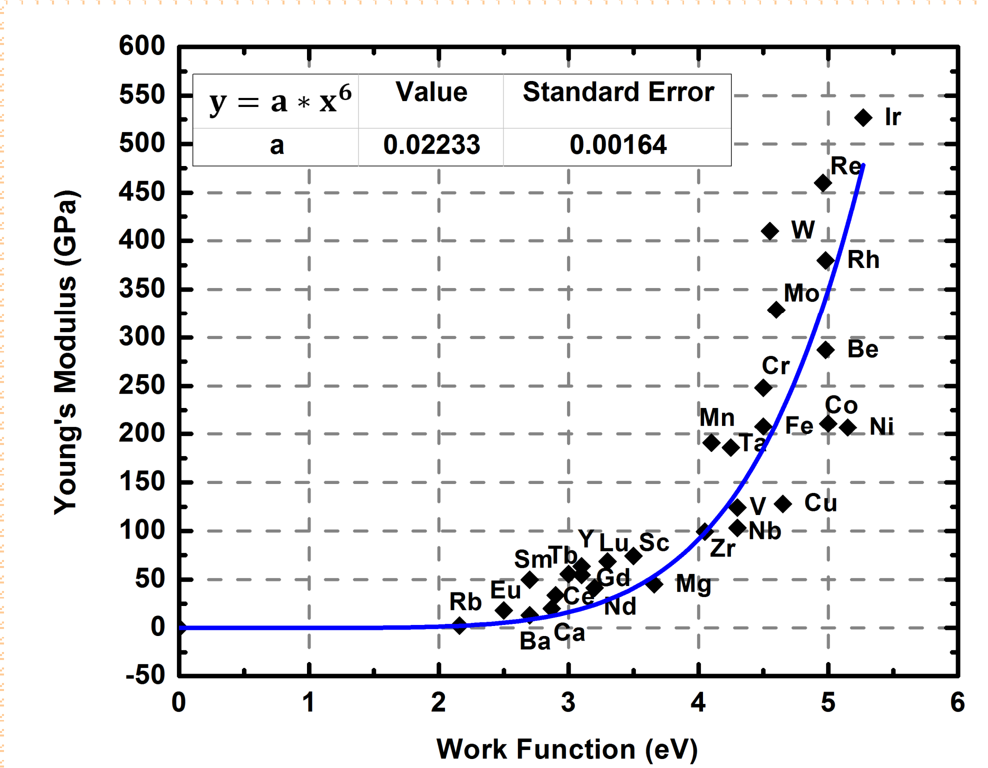


Scanning Kelvin Probe

2. Correlation between EWF and properties of materials

- Young's modulus

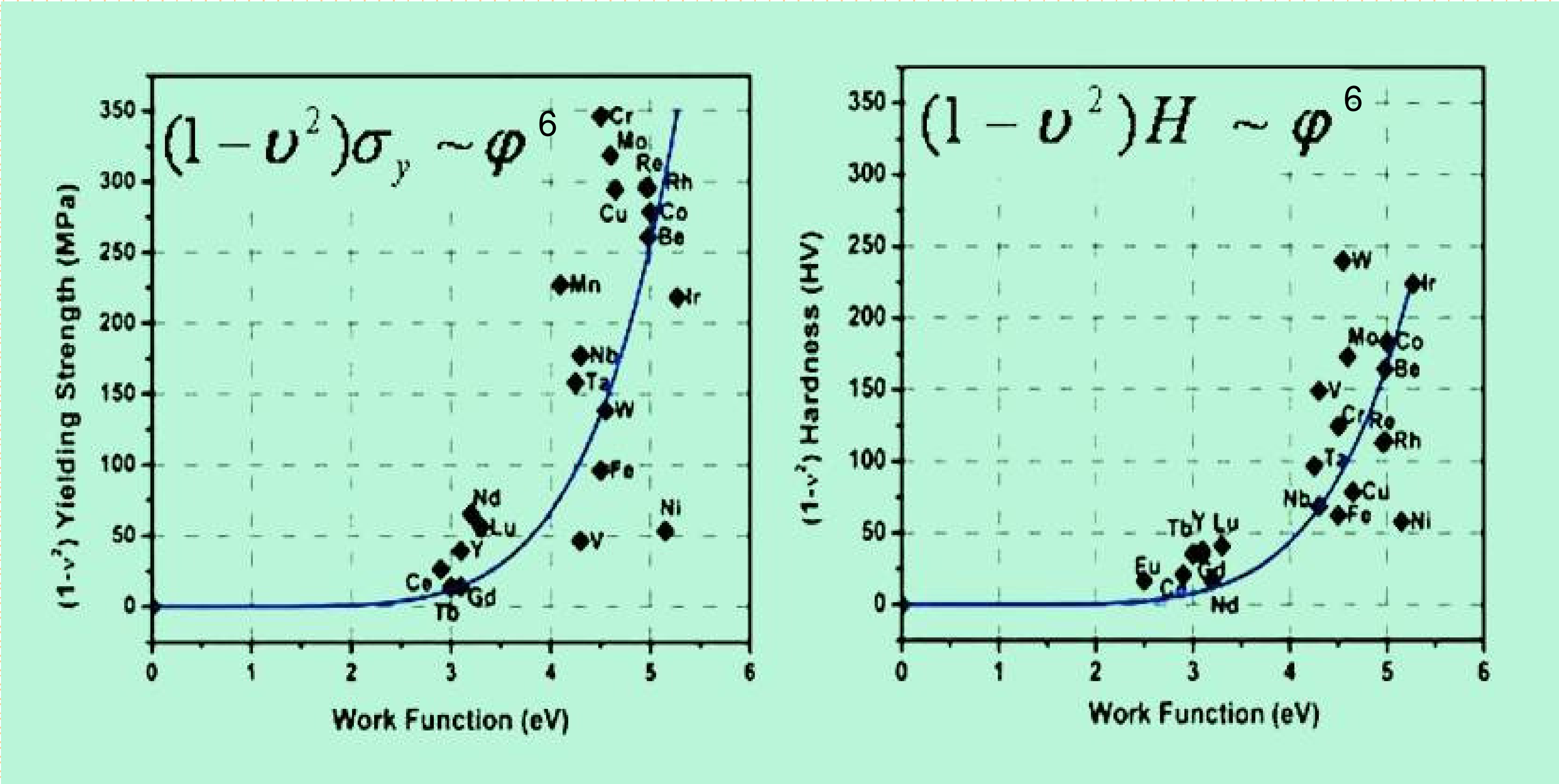
$$E = 2\alpha e^{2}\left(\frac{16\sqrt[3]{3}\,\pi^{\frac{5}{3}}\hbar\varepsilon_0^{\frac{3}{2}}}{e^{3}m^{\frac{1}{2}}}\right)^{6}\varphi^{6} = \alpha\frac{18\times 16^{6}\pi^{10}\hbar^{6}\varepsilon_0^{9}}{e^{16}m^{3}}\varphi^{6} \propto \alpha\varphi^{6}$$



The higher the EWF, the stronger the material (harder to change the electron state).

Guomin Hua and D.Y. Li, Generic Relation between the Electron Work Function and Young's Modulus of Metals, **Appl. Phys. Lett.**, 2011, DOI: 10.1063/1.3614475

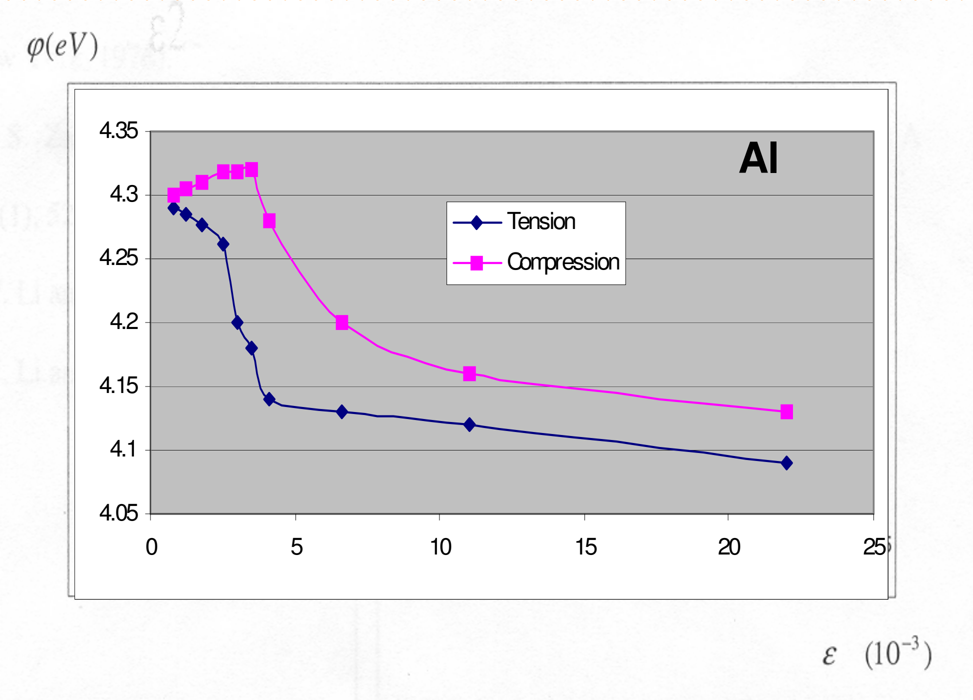
- Yield strength and hardness

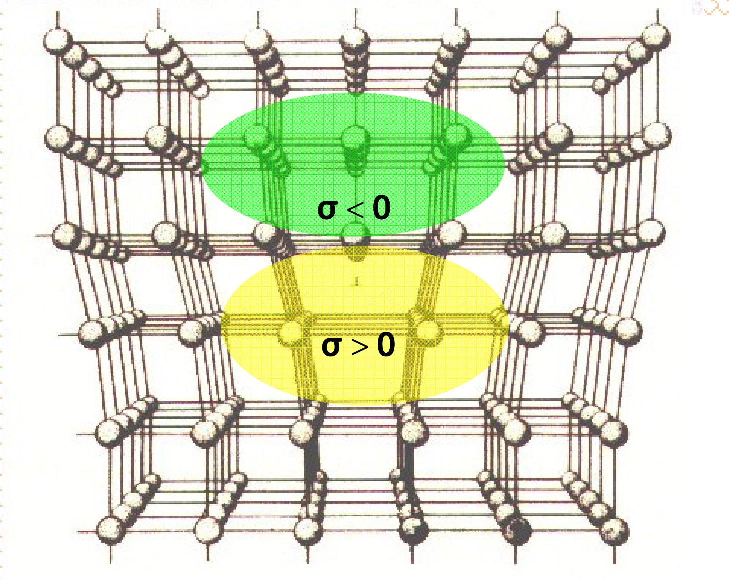


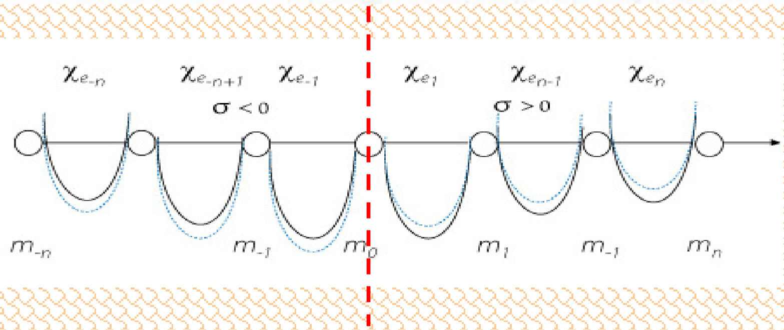
υ - Poisson ratio

Guomin Hua and Dongyang Li, The correlation between the electron work function and yield strength of metals, **Phys. Status Solidi (b)** 249 (2012) 1517–1520.

- Deformation behavior





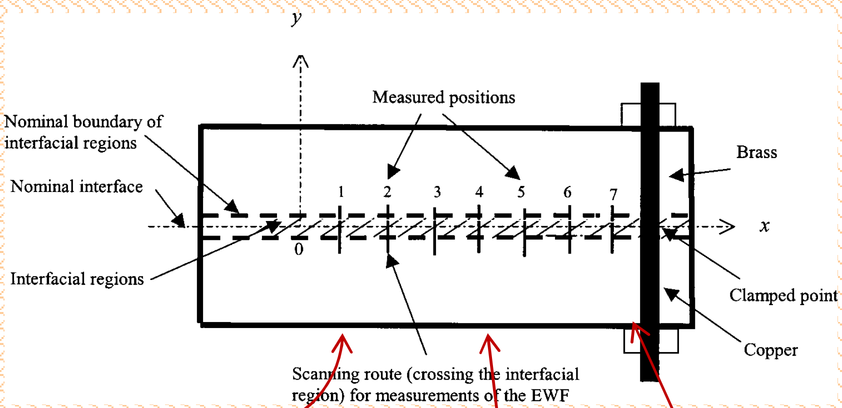


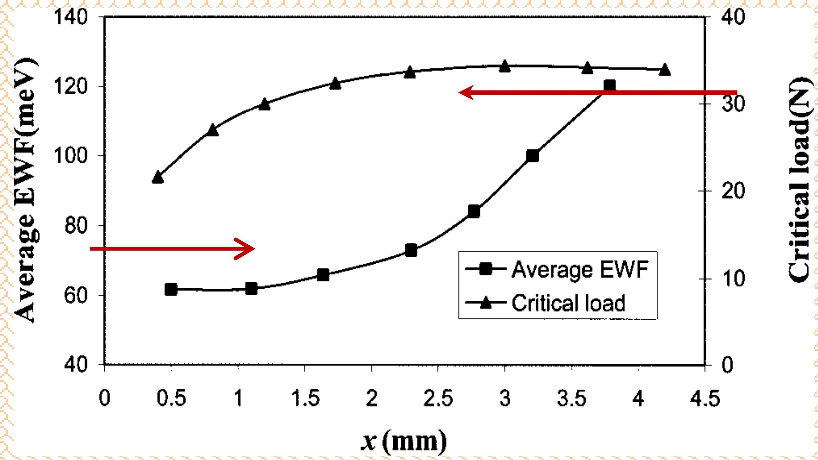
The potential well depth varies as stress is applied and this leads to changes in *EWF*. Both elastic and plastic deformations can be reflected by changes in *EWF*.

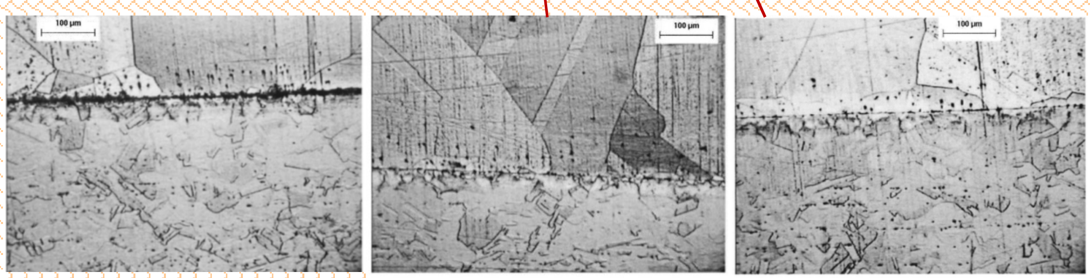
D.Y. Li, Kelvin probing technique: a promising method for determination of the yield strain of a solid under different types of stress, **Phys. Stat. Sol. (a)**, 191 (2002) 427.

W. Li, D.Y. Li, Effects of Dislocation on the Electron Work Function of a Metal Surface, **Mater. Sci. & Tech.**, 18 (2002) 1057.

- EWF and interfacial bonding strength







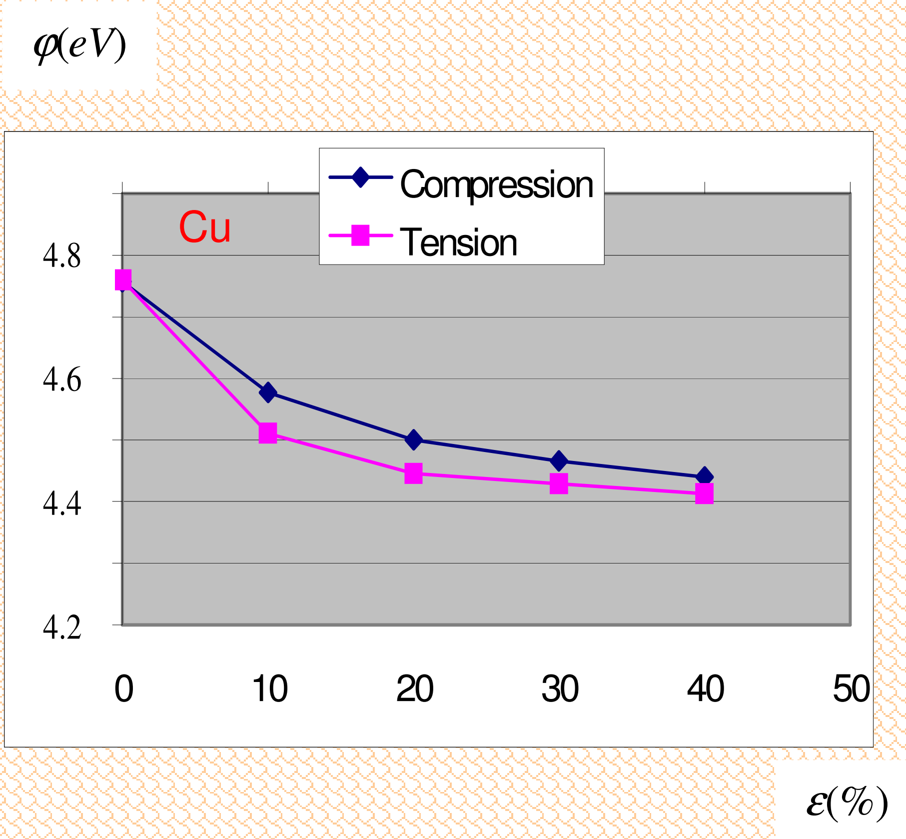
Variations of the critical load and the average EWF of interfacial regions with respect to change in interfacial position from 1 to 5.

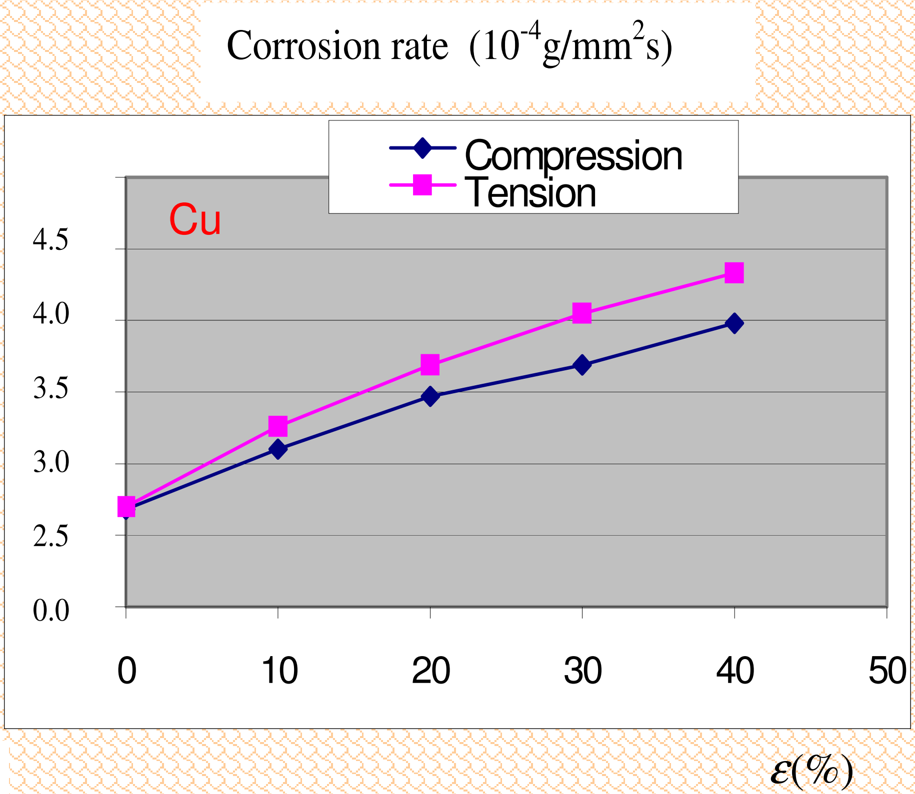
Schematic of the formation of an interface – annealing clamped two pieces of Cu and brass (diffusion treatment for bonding)

The higher the interfacial EWF, the stronger the interfacial bonding (harder to change the interfacial electron state).

W. Li and D.Y. Li, **J. Appl. Phys.**, 97, 014909 (2005).

- EWF and corrosion



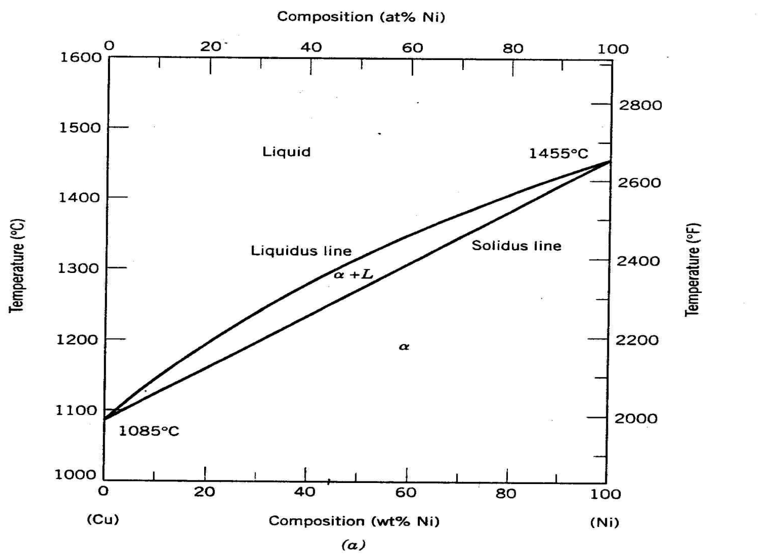


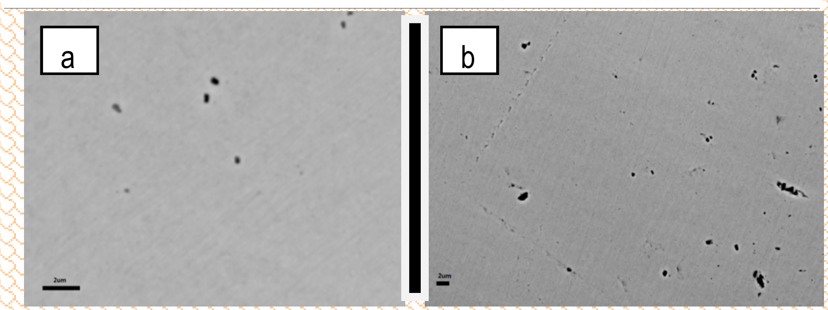
Plastic deformation makes materials more anodic and thus less corrosion resistant.

W. Li, D.Y. Li, **Appl. Surf. Sci.,** 240 (2005) 388-395.

3. Can EWF be a design parameter for materials?

- EWF and properties of Cu-Ni alloys





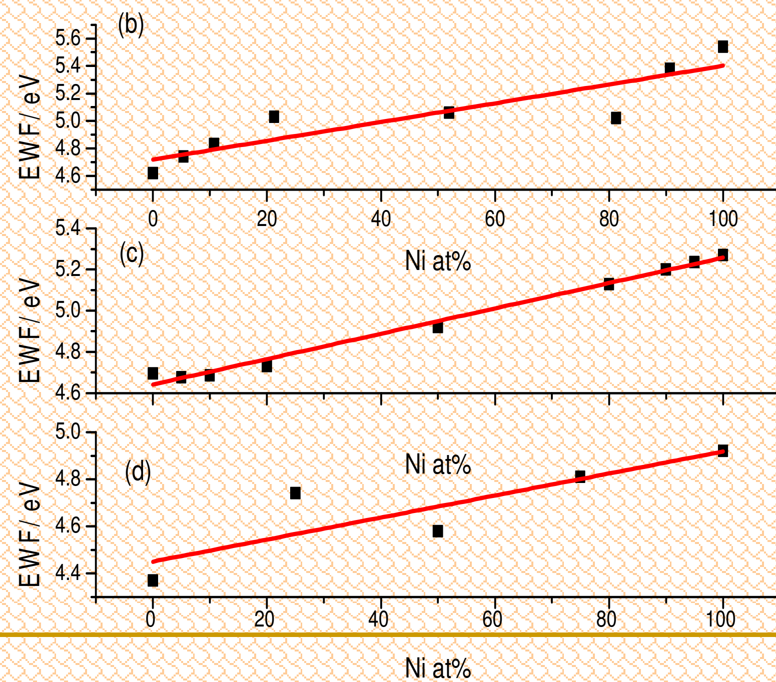
SEM backscattered images of samples with 90 wt% Ni (a) and 20 wt% Ni (b).

For binary isomorphous solutions

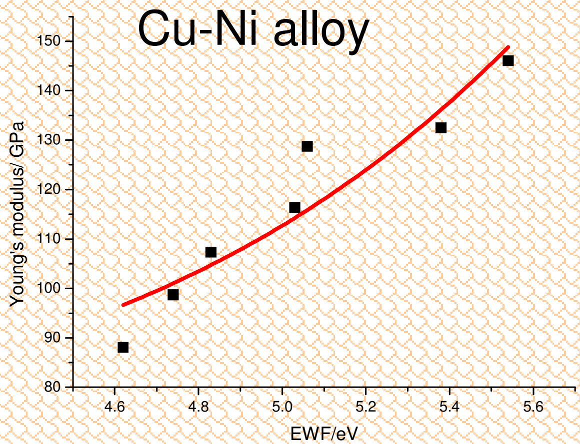
$$\varphi_{AB} = X_A \varphi_A + (1 - X_A)\varphi_B$$

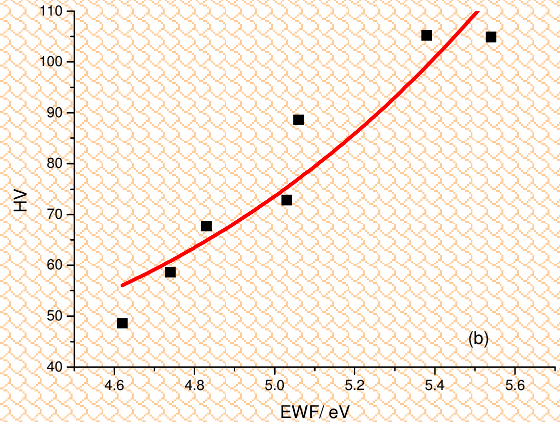
X_A – Molar fraction of element A

$\varphi_{Cu} \approx$ 4.6 eV $\qquad$ $\varphi_{Ni} \approx$ 5.2 eV

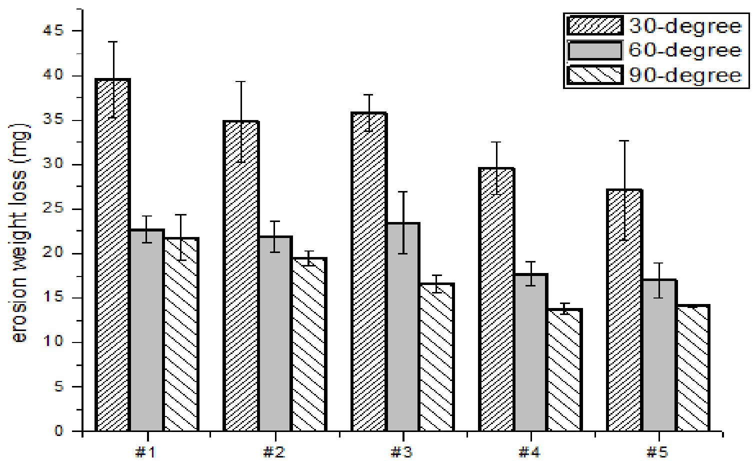


H. Lu, G. Hua, and DY Li, Appl. Phys. Lett., 103, 261902 (2013)





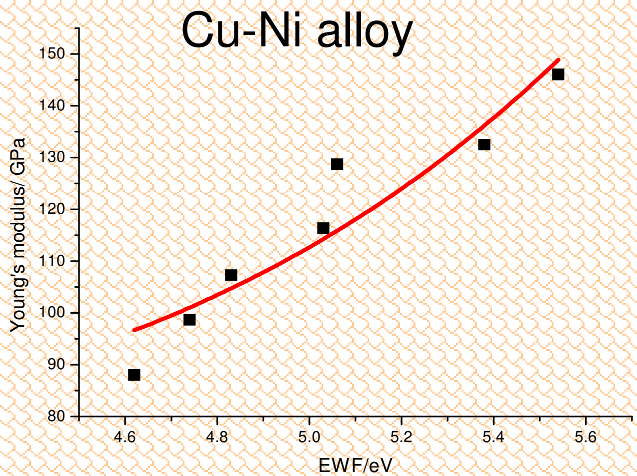
$\varphi \uparrow \Rightarrow$ Strength $\uparrow$



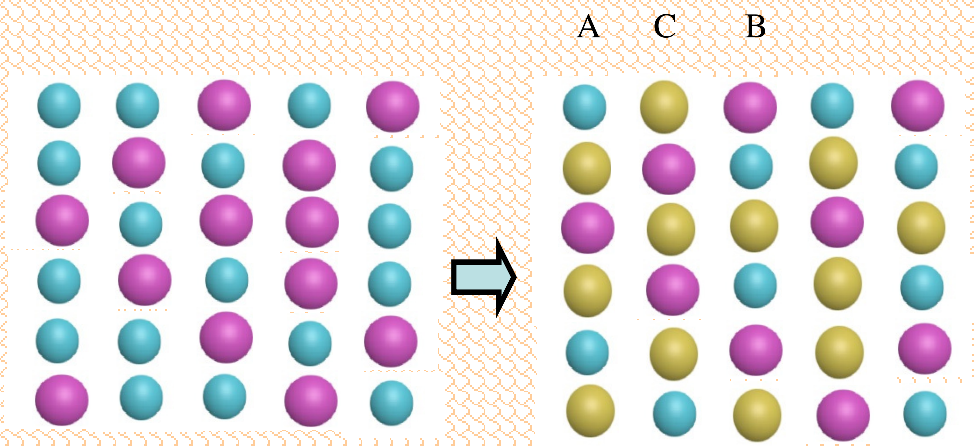
Sample NO.	Cu content (wt. %)	Ni content (wt. %)
#1	100	0
#2	80	20
#3	50	50
#4	20	80
#5	0	100

$$Erosion \propto \frac{mV^2}{H}$$

Erosion rates of the fabricated alloys at three impingement angles.



$\varphi \uparrow \rightarrow$ Strength $\uparrow$



Schematic illustration of a configuration in which a portion of A-A, B-B and A-B bonds are replaced by A-C, B-C and C-C bonds when a third element, C, is added.

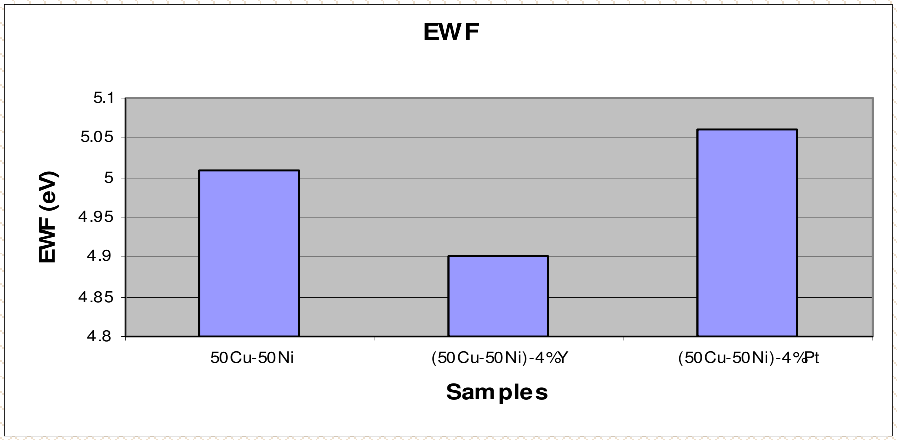
Logically, adding an element having a higher work function to a host metal may raise the overall work function and could thus enhance the atomic bonding and consequently the mechanical strength of a bulk material, an interface, or a surface.

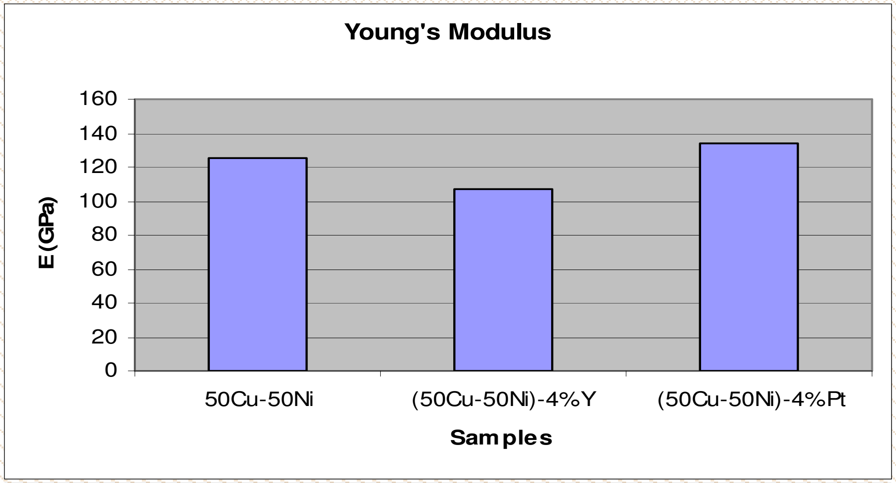
- Selection of elements for solution-hardening based on EWF

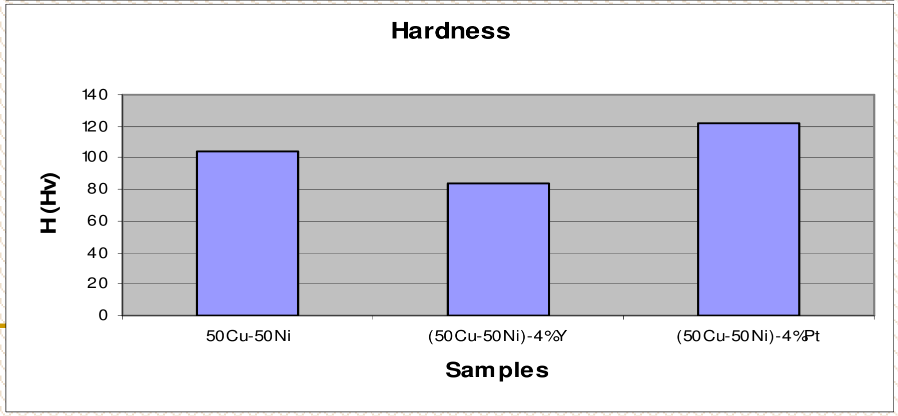
50Cu-50Ni: EWF=5.01 eV
Yttrium: EWF= 3.1eV
Platinum: EWF=5.32-5.65 eV

50Cu-50Ni with Y	0%wt Y	4%wt Y
EWF (eV)	5.01	4.90
50Cu-50Ni with Pt	**0%wt Pt**	**4%wt Pt**
EWF (eV)	5.01	5.06

A higher work function corresponds to a more stable state with a higher resistance to attempts of changing the state

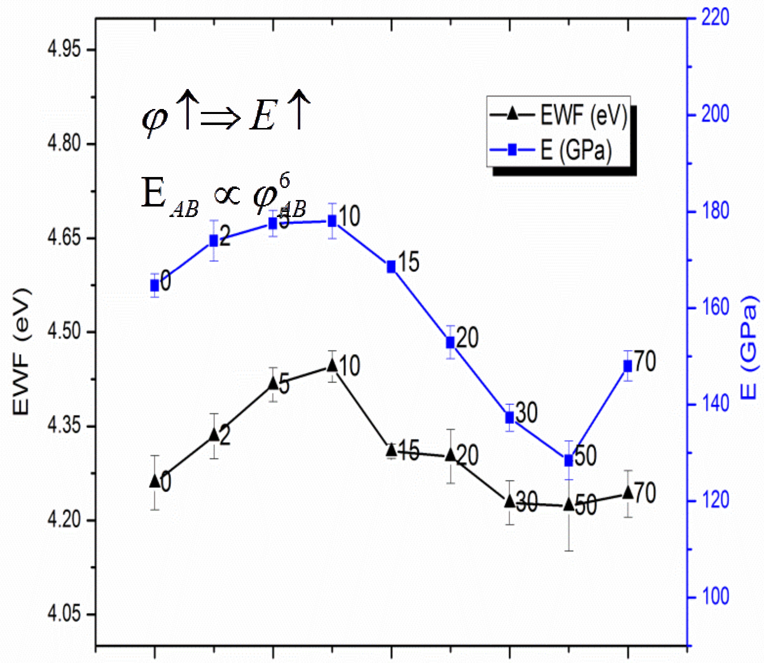


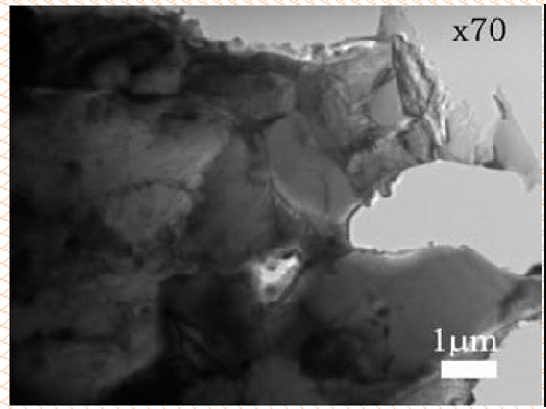


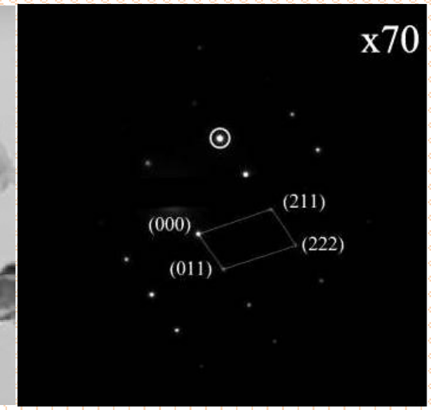


- EWF and properties of multi-phases alloys

e.g., X70 pipeline steel (0.066 wt% C, 0.5 wt% Mn, 0.3 wt% Cr) + Ni







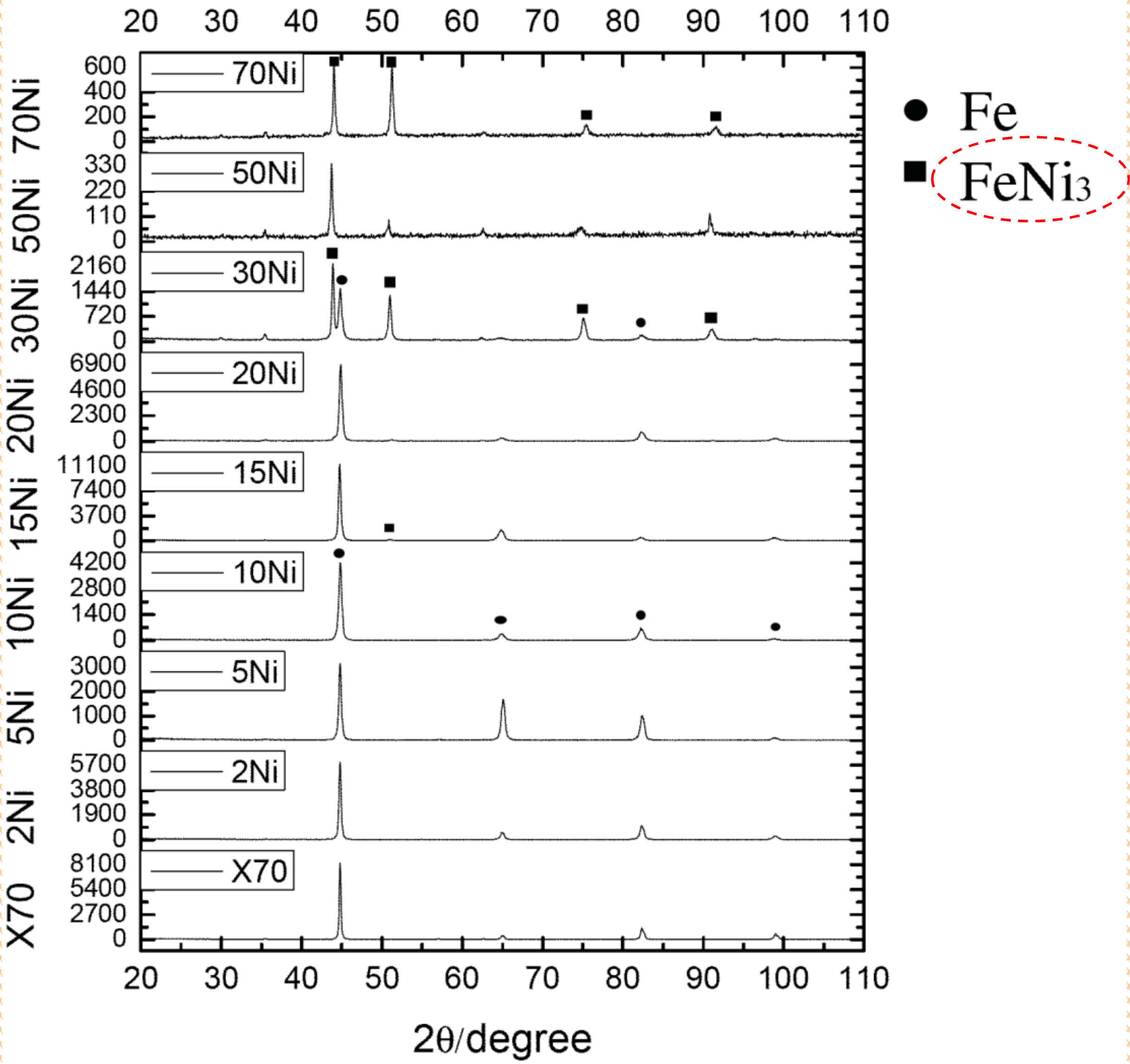
Ni more than 10 wt%, both EWF and Young's modulus decrease.

Why?

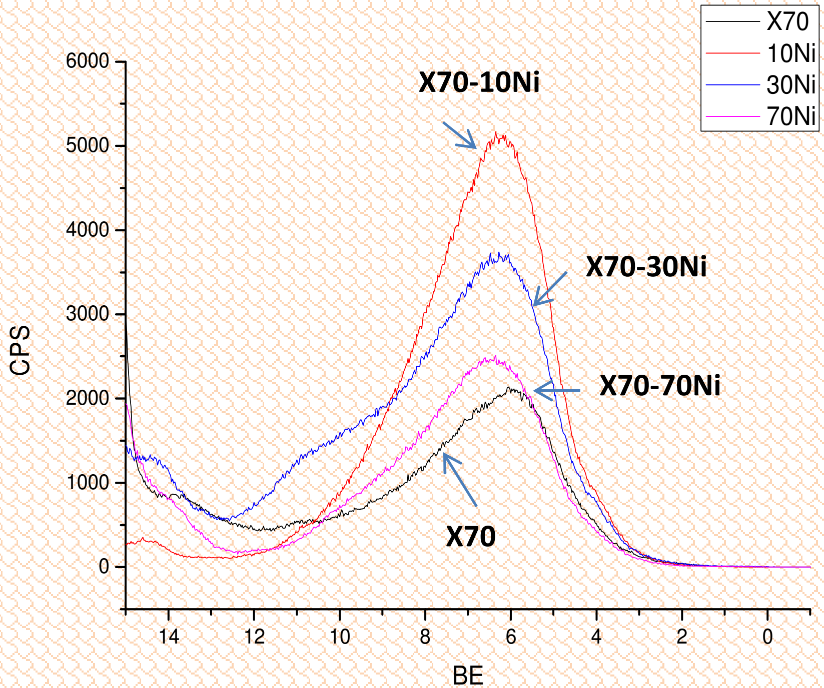
$\varphi_{Ni} = 5.15eV \quad \varphi_{Fe} = 4.5eV$

	E (GPa)	HV	EWF (eV)
X70	164.7	190.7	4.260
X70-2Ni	174	259.4	4.334
X70-5Ni	177.6	266.5	4.416
X70-10Ni	178.1	319.7	4.445
X70-15Ni	168.6	304.4	4.310
X70-20Ni	152.9	282.6	4.302
X70-30Ni	137.3	114.4	4.228
X70-50Ni	128.4	112.5	4.223
X70-70Ni	148.0	136.3	4.242

Phases and %Ni



“Free” electron density and strength



Valence electron density of Ni-X70 samples

$$\varphi \propto n^{1/6} = z^{1/6} / a^{1/2}$$

Second phases may change the number of available free electrons and consequently the overall electron density.

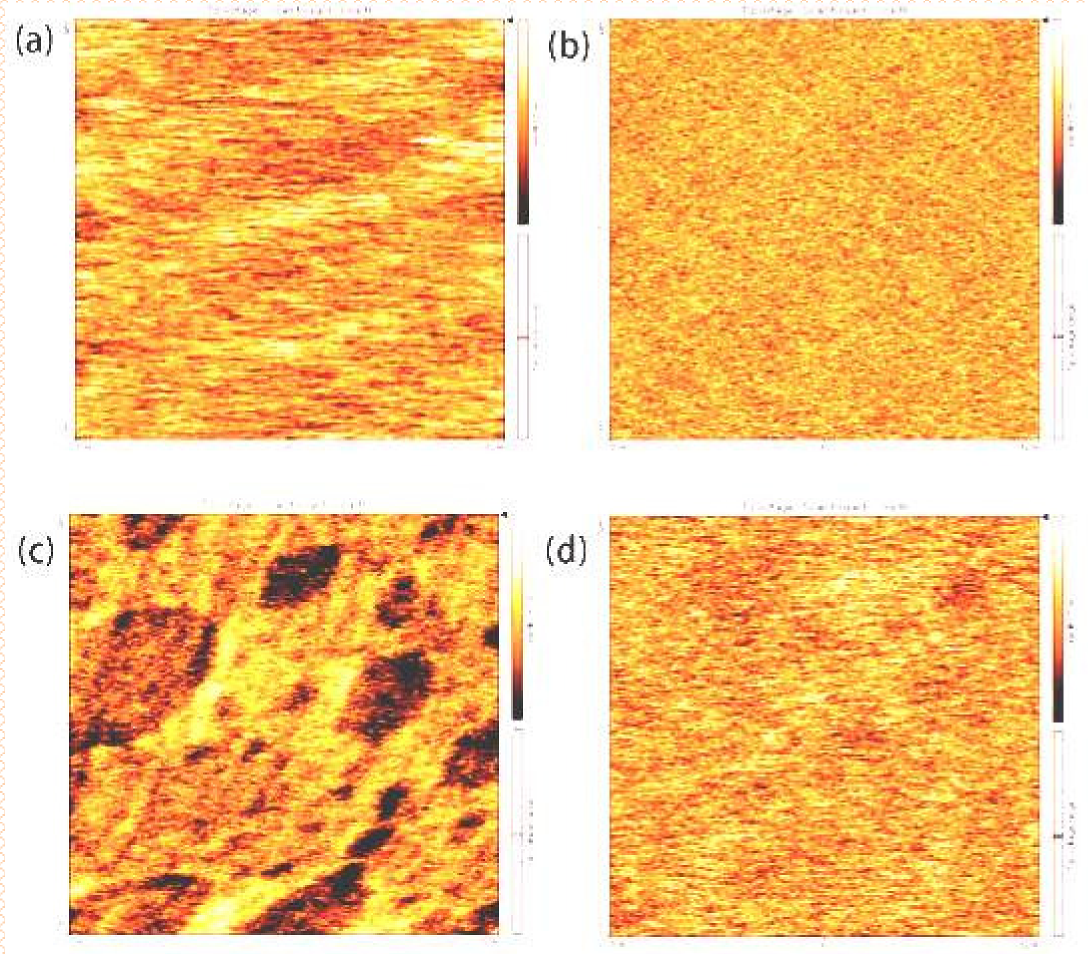
	B (GPa)	G (GPa)	E (GPa)
Fe	178.3	79.5	207.9
Ni	180.4	86.2	223.1
$FeNi_3$	173.0	69.8	184.5

$$Hv \propto G$$

$$Hv \propto G\left(G/B\right)^2$$

Why X70-30Ni softer?

EWF mapping



Work function maps of (a) X70, (b) X70-10Ni, (c) X70-30Ni, (d) X70-70Ni given by AFM. Darker regions represent lower work function.

$$\varphi_{FeNi_3} < \varphi_{X70-70Ni} \leq \varphi_{X70} < \varphi_{X70-10Ni}$$

4. Conclusions

- EWF is a fundamental parameter that is directly related to mechanical, physical and chemical properties of materials.

- EWF helps to get an insight into various material-related processes.

- EWF can be a simple but fundamental parameter for material design.

Acknowledgement

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  Dr. Z.R. Liu, PDF

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