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## Electronic Transport in Alloys

*A criterion for true physics is the correspondence between theory and experiment. Two other criteria are beauty and symmetry of the underlying formulas - formulas (2) and (6).*

**Key words:**

Hall effect, Giant Hall effect,  
Seebeck coefficient (Thermopower),  
Electron density,  
Conductivity,  
Ioffe-Regel criterion,  
Minimum metallic conductivity,  
Composites, Nanocomposites

In the field of solid state physics, there are a number of unanswered questions that have stubbornly resisted scientific explanation for decades.

***These questions are:***

1) Why are there simple metals with *positive* thermopower, even though, according to theory, the

thermopower of simple metals should always be negative?

2) What is the reason for the phenomenon of the "*Giant Hall effect*" in metal-insulator composites?

3) Why can amorphous metal films exist at all, even though the crystalline state is the more stable?

4) Is there a Minimum metallic conductivity  $\sigma_{min}$ ?

5) Why does the electrical conductivity  $\sigma$  of a metal film decrease exponentially with decreasing film thickness? (Proximity effect)

6) Superconductivity of thin films - Why do superconductors as a thin film often have a higher transition temperature  $T_S$  than their compact counterparts?

During the study of publications on the standard theory of electron structure and electronic transport phenomena in disordered alloys (N. F. Mott, P. W. Anderson, U. Mizutani and others) I noticed contradictions between the experimental findings and the theoretical predictions. So I suspected that the theory might be inaccurate or wrong. By thoroughly analyzing the existing experimental  $\sigma$  data, I discovered for amorphous metal-metalloid alloys a simple mathematical relationship between  $\sigma$  and  $x$ , the metalloid content in the alloy:  $\sigma \propto \exp[x/(1-x)]$ . On the basis of this finding, I formulated a physical model that directly relates the electron structure in these alloys to its topological structure. The crucial thing in this model is that these amorphous alloys are considered to be *nanocomposites* in which different phases with different structures coexist. Nanocomposite bedeutet eine Mischung verschiedener Phasenkörner, deren Abmessungen im Nanometerbereich liegen. Nanocomposite means a mixture of different phase grains, the dimensions of which are in the nanometer range. This view was later experimentally confirmed (A. Bienenstock, M. J. Regan, R. D. Lorentz und andere, Zitate 28 bis 32 in Phys. Rev. **B 71**, 115114 (2005)). The formulas (5), (9), (10) and (11) (see below) follow directly from this physical model. This led to the question: Can the other electronic parameters such as Seebeck coefficient (Thermopower)  $S$  and Hall coefficient  $R$ , be derived mathematically from this model? The questions were therefore:

- 1) How to calculate  $S$  from the known  $S_i$  values?
- 2) How to calculate  $R$  from the known  $R_i$  values?

The theory already provided formulas for this, but these also proved to be incomplete or incorrect on closer analysis. What these errors consist of is addressed in the review article: J. Sonntag, B. Lenoir and P. Ziolkowski, *Electronic Transport in Alloys with Phase Separation (Composites)*. Open Journal of Composite Materials, 2019, 9, 21-56 [www.scirp.org/Journal/PaperInformation.aspx?PaperID=90216](http://www.scirp.org/Journal/PaperInformation.aspx?PaperID=90216)

The new, corrected formulas for  $S$  and  $R$  are the formulas (1), (2), (6) to (8).

In the above-mentioned review article, the derivatives for formulas (1) to (8) are again justified.

This new physical model with its formulas also provides answers to the questions 1) to 6) listed above.

### ***The answers to the questions:***

The answer to 1) is given by the formula (4). The classic formula  $S_0$  always provides negative thermopower. The new formula (4) provides positive thermopower, when the second term is positive and if it dominates the first. Examples are Cu, Ag, Au, Li. (4) follows as limiting case of (2) for an one-phase alloy, i.e.,  $v_A \rightarrow 0$ .

The answer to 2) is given by the formula (5) in connection with (6).

The answer to 3) is given by the formula (5).

The answer to 4) is: YES. This answer is given by the formulas (10) and (11), both of which follow from formula (9).

The answer to 5) is given by the formula (5) in conjunction with the fact that the loss of electrons in the thinner metal film (by electron transfer to the substrate occupying surface states) is distributed over fewer metal atoms than in thicker metal films. Therefore, the electron density in the metal film decreases as the thickness of the metal film decreases. Exponential, because the application of formula (5) leads to an exponential dependency.

The answer to 6) is given by formula (5), because the formation of the Cooper pairs depends also on the electron density.

## **The second most beautiful formulas in physics:**

### **Thermopower (Seebeck coefficient) for alloys with phase separation (*composites*)**

$$\sum_i v_i \frac{\sigma_i/S_i - \sigma/S}{\sigma_i/S_i + 2\sigma/S} \approx 0 \quad (1)$$

$$\sum_i v_i \frac{\kappa_{e,i}/S_i - \kappa_e/S}{\kappa_{e,i}/S_i + 2\kappa_e/S} = 0 \quad (2)$$

where  $S_i$  is given by

$$S_i = S_{i,0} + \frac{1}{|e|} \frac{d\mu}{dT}. \quad (3)$$

### **Thermopower in *homogeneous* alloys**

$$S = S_0 + \frac{1}{|e|} \frac{dE_c}{dT} \quad (4)$$

— **Electron density in alloys with *amorphous***

***phase separation* (electron transfer between the phases)**

$$dn = -\beta \cdot n \cdot d\zeta \quad (5)$$

### **Hall coefficient formula for *two-phase composites***

$$R = \frac{\sigma_A^2 R_A [\sigma_B + \sigma(3v_A - 1)] + \sigma_B^2 R_B [\sigma_A + \sigma(3v_B - 1)]}{\sigma(\sigma_A \sigma_B + 2\sigma^2)} \quad (6)$$

### **General Hall coefficient formula for *composites* with two or more phases**

$$\left( R\sigma^2 \frac{\partial}{\partial \sigma} + \sum_i R_i \sigma_i^2 \frac{\partial}{\partial \sigma_i} \right) f(\sigma, \sigma_i) = 0, \quad (7)$$

where

$$f(\sigma, \sigma_i) = \left( \prod_i (\sigma_i + 2\sigma) \right) \left( \sum_i v_i \frac{\sigma_i - \sigma}{\sigma_i + 2\sigma} \right) \quad (8)$$

### **Ioffe-Regel criterion (*Alternative interpretation*)**

$$k_F L \geq c^* = \frac{1}{4} \quad (9)$$

### **Minimum metallic conductivity; *strong scattering***

$$\sigma_{min} = \frac{c^{*2}}{6} \left( \frac{e^2}{h} \right) \frac{1}{d} = \frac{1}{96} \left( \frac{e^2}{h} \right) \frac{1}{d} \quad (10)$$

### **Minimum metallic conductivity; *general case***

$$\sigma_{min} = \frac{2c^{*2}}{3\pi} \left( \frac{e^2}{h} \right) \frac{1}{L} = \frac{1}{24\pi} \left( \frac{e^2}{h} \right) \frac{1}{L} \quad (11)$$

### **The formulas (1)-(11) I have published in:**

- (1): Phys. Rev. **B 73**, 045126 (2006)  
 (2): J. Phys.: Condens. Matter **21** (2009) 175703 and J. Mater. Chem. C, **4**, 10973 (2016)  
 (3),(4): J. Phys.: Condens. Matter **22** (2010) 235501  
 (5): Phys. Rev. **B 40**, 3661 (1989)  
 (6)-(8): Open J. of Composite Materials **6** (2016) 78  
 (9): Phys. Rev. **B 71**, 115114 (2005) (Appendix)  
 (10),(11): Phys.Rev.**B73**, 045126 (2006) (Appendix B)

$S$  - Seebeck coefficient

$R$  - Hall coefficient

$\sigma$  - electrical conductivity

$\kappa_e$  - electronic contribution to the thermal conductivity  
 $S_i$ ,  $R_i$ ,  $\sigma_i$ ,  $\kappa_{e,i}$  and  $v_i$  are the Seebeck coefficient, Hall

coefficient, electrical conductivity, electronic contribution to the thermal conductivity, and volume fraction, respectively, of the individual phase  $i$  [ $i = A, B, \dots$ ].

$S_0$  and  $S_{i,0}$  are the *classical* thermopower formula for a homogeneous alloy and for the phase  $i$ , respectively.

$n$  - electron density [in a two-phase composite  $n$  is the electron density in the phase with the higher potential ( $\equiv$  phase  $A$ )]

$\zeta = v_B/v_A$

$\beta$  - a constant for a given alloy, which is determined by the average potential difference between the two phases.

$E_c$  - band edge of the conduction band

$T$  - temperature

$\mu$  - electrochemical potential

$k_F$  - wave number at the Fermi surface

$L$  - mean free path of the electronic carriers

$d$  - average atomic distance