



Regular Article

A general formulation for solid solution hardening effect in multicomponent alloys



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ARTICLE INFO

Article history:

Received 4 July 2016

Received in revised form 24 August 2016

Accepted 8 September 2016

Available online xxxx

Keywords:

High entropy alloys

Metal and alloys

Hardness

Yield phenomena

Modeling

ABSTRACT

This paper presents a general formulation for the effect of the solid solution hardening (SSH) in multicomponent alloys. It bridges the existing approaches analyzing this hardening effect between binary alloys and highly concentrated multicomponent systems. The model is validated with a comprehensive dataset of measured critical resolved shear stress, hardness and yield strength of binary and multicomponent systems from the literature.

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High entropy alloys (HEAs) are one of the most proposing new materials for key industrial applications. Especially where a combination of properties such as microstructural stability, mechanical properties at high temperature, corrosion, oxidation and/or radiation resistance [1], is required. The number of possible compositional combinations to test experimentally is immense, although just a minor fraction will probably be a solid solution. This has stimulated large efforts to develop models and parameters able analyze millions of compositions and prioritize which compositions could be a HEA [2]. Among the minor fraction (still large in number) of alloys being HEAs, certainly not all of them will have interesting industrial properties. Nevertheless, the physical models able to predict the properties of those alloys are still on development. The use of existing models, valid for existing alloys where one of the elements dominate over the others, can be used as a guide for modeling generalize highly concentrated multicomponent systems, such as the HEAs, but they need to be adapted or extended due the cocktail effect and the large lattice distortion in this alloys [3].

A first attempt to describe the solid solution hardening (SSH) effect in multicomponent systems, one of the largest effect on yield strength in HEAs, was done at Ref. [4]. In that work, a relative success was achieved by using the approaches proposed by Fleischer

and Labush for binary systems [5,6], and adapting the extension to multicomponent alloys proposed at Ref. [7]. One of the key parameters in these models was the calculation of the unit cell parameter of the alloy and its variation with composition. In that work [4], the model for calculating the unit cell parameter proposed by Lubarda for binary interactions was applied [8]. More recently, the use of a matrix describing the lattice distortion, originally proposed for binary systems for this purpose [9], was extended for multicomponent alloys [10]. This matrix, and the methodology developed at Ref. [10] is used here to replace the abovementioned Lubarda's approach for the unit cell parameter calculation, and allows the computation of both the lattice parameter and its variation with composition, as well as other important parameters related to the crystal stability in HEAs [11]. This methodology is used in this work to develop a model that generalizes the proposed approach [4] for multicomponent alloys.

The SSH effect, in binary or multicomponent alloys, is due to the variation in the lattice coordinates with respect to ideal positions induced by the presence different elements. In the original works [5,6], this effect is accounted by the solute–solvent interaction, while in the present work, it is based on the lattice distortion due to the presence of different elements. While both philosophies can be applied to dilute alloys, the proposed one here is intended to describe the large complexity of interactions of multicomponent alloys, but being also consistent with binary systems.

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The original formulation for binary systems [6] proposes that the SSH effect $\Delta\sigma_{ss}$ is:

$$\Delta\sigma_{ss} = B x^{2/3} \quad (1)$$

being x the solute content and B :

$$B = 3\mu Z \left[\xi(\eta^2 + \alpha^2 \delta^2)^{1/2} \right]^{4/3}, \quad (2)$$

where μ is the shear modulus of the alloy, Z is a constant and α is a parameter that accounts for the difference in the interaction forces between screw and edge dislocations and the solute atom, where it is assumed that $3 < \alpha < 16$ for screw dislocations and $\alpha > 16$ for edge dislocations [12], ξ it is related to the activated slip systems in different crystal structure, η' and δ are the elastic misfit and atomic size misfit respectively, and the multiplier 3 stands for the Taylor factor [6]. For a general model, it is usually taken $\alpha = 16$ [4] since it accounts for a mixture of dislocations type in the material, and the constant Z has been experimentally fitted to $Z = 5$ in this work. The calculation of the shear modulus of the alloy is described in Ref. [11] and it is based on the use of the elemental unit cell parameter and elastic constants. Similarly, a simple mixing rule of the elemental shear modulus with the corresponding atomic fraction [4] provides a similar approximation to the shear modulus of the alloy. For simplicity, each elemental shear modulus is taken for each element at its respective crystal structure. Although the shear modulus changes with crystal structure, it has been seen that variations in the range of 2–5% for phase transitions can be expected [13], where the effect of microstructure is ignored here since elastic properties have been observed to mostly depend on composition [14]. Being both misfits of similar magnitude and due to the large value of α , the parameter ϵ can be approximated by $\epsilon \approx \xi \alpha |\delta|$, and then Eq. (2) is simplified to:

$$B = 3\mu Z (\xi \alpha |\delta|)^{4/3}, \quad (3)$$

where, finally, the atomic size misfit δ is defined as:

$$\delta = \frac{da}{dx} \frac{1}{a} \quad (4)$$

with a the unit cell parameter of the alloy.

This formulation was developed for a medium concentration of solutes by Labush [6], experimentally validated for concentrations mostly around 0–20 at.%, and extends the original formulation for the hardening effect of dilute binary alloys [5]. In both approaches, Eq. (4) stands for the local variation of the cell parameter by means of the effect of isolated solutes. These solutes were assumed to not interact to each other, which is not the case of highly concentrated solid solutions. For a highly concentrate binary alloy with elements type i and j , even if element i is dominant, the effect of atom of type j (solute) in atom of type i (solvent) can be as large as its reciprocal, the effect of atom i in atom of type j . A logical choice to account for this effect is to adopt a matrix form of the solid solution hardening effect $\Delta\sigma_{ss}^m$ that generalizes Eq. (1) for low solute concentrations. If $x = x_j$ is the concentration of the solute and $x_i = 1 - x_j$ the solvent, this has the form:

$$\Delta\sigma_{ss}^m = Bx^{2/3}(1-x)^{2/3} = \frac{1}{2} \begin{pmatrix} x_i^{2/3} & x_j^{2/3} \end{pmatrix} \begin{pmatrix} 0 & B \\ B & 0 \end{pmatrix} \begin{pmatrix} x_j^{2/3} \\ x_i^{2/3} \end{pmatrix}. \quad (5)$$

Indeed, for very low solute concentration $\Delta\sigma_{ss}^m \approx \Delta\sigma_{ss}$, since $(1-x)^{2/3} \approx 1$, but it quickly differs from the original formulation for concentration x still in the range of applicability of Labush's approach.

An alternative is to assume that the parameter B , which accounts for the effect of i on j and vice versa, applies by the frequency of possible i - j interactions, which is $x_i x_j$, or $x(1-x)$ if using the original formulation for binary systems. It is assumed that the i - i and j - j interactions, with frequency of occurrence $x_i x_i$ and $x_j x_j$ respectively, does not affect the solid solution hardening effect, in concordance with Labush's approach. Then, the following formulation much simpler is proposed:

$$\Delta\sigma_{ss}^m = 2Bx(1-x) = (x_i, x_j) \begin{pmatrix} 0 & B \\ B & 0 \end{pmatrix} \begin{pmatrix} x_j \\ x_i \end{pmatrix}. \quad (6)$$

The range of applicability of this formulation is intended for high concentrations, but it needs to be consistent with the existing formulation for dilute solid solutions. The performance of Eqs. (5) and (6) to approximate Eq. (1) is depicted in Fig. 1 for the same value of B . It can be observed in that figure that Eq. (5) is just valid for very diluted concentrations, while Eq. (6) is more consistent with Eq. (1). It is also based on a more convincing effect of element i on element j and vice versa by means of the frequency of occurrence of their interaction.

In highly concentrated alloys, such as the HEAs, there is not a reference solvent element, since all elements are in similar content and the concept of solvent and solute vanishes. The local variation of the cell parameter in the crystal lattice, which is the responsible of the hardening effect, remains and is due to the different local combinations of elements in the crystal lattice. This effect is known as the distortion in the lattice, and a formulation to describe it was proposed at Ref. [10]. We will use the concept of the lattice distortion, rather than the solute-solvent interaction, to explain the hardening effect in highly concentrate alloys. Eq. (6) is convenient for this purpose, since it does not distinguish between solute-solvent, but it can be also applied to low concentrated alloys.

The approach to account for the lattice distortion is based on the use of the interatomic spacing matrix $S = \{s_{ij}\}$, proposed initially by Moreen [9], which accounts for the mean value of the distribution of interatomic spacing distances, also called nearest neighbor distances, between atoms of different species in the alloy. Each individual interaction distance between atoms of type i and j can fluctuate over a range of values, depending on the combination of atoms and its coordinates around i and j . The averaged value of all i - j distances is captured by s_{ij} in matrix S . The matrix S is related to the mean interatomic spacing of the alloy s_{lat} by the frequency of occurrence of each i - j interaction. The contribution to the mean interatomic distance across the lattice by i - j interactions is therefore $s_{ij} x_i x_j$, where x_i and x_j

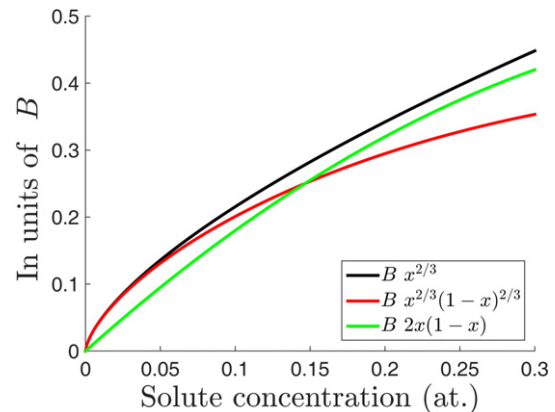


Fig. 1. Comparison of different solid solution hardening effect formulations for binary systems by means of the solute content x and $B = 3Z\mu\left(\frac{\xi\alpha}{a}\frac{da}{dx}\right)^{4/3}$.

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