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Solid solution strengthening theories of high-entropy alloys

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Abstract

We present a review of solid solution strengthening models for random concentrated solid solutions of which high entropy alloys are an interesting subset. High entropy alloys (HEAs) usually refer to a class of multicomponent alloys in equal or near equal concentrations. These complex compositions break the conventional notion of solutes and solvents. Few attempts have been made to extend the conventional solute strengthening models to HEAs. Among these, the model based on an average effective medium, does not include any adjustable parameter, allows all model inputs to be computed by atomistic simulations, and has predicted the strength of fcc HEAs in good agreement with experiments. The basic concepts of this theory is explained and its capabilities are compared with few other existing models for solute strengthening of HEAs.

^a CRL and MS made equal contributions to this work.

INTRODUCTION

The term “high entropy alloy” (HEA), coined by Yeh *et al.*, refers to a relatively new class of multicomponent alloys, usually five or more components, in equal or near equal concentrations [1]. Instead of the ordered intermetallic phases expected from classical physical metallurgy, some HEA systems strikingly crystallize as single phase solid solutions with simple crystal structures [2–6]. The initial reasoning for the formation of HEAs was that the high configurational entropy would tend to stabilize solid solution formation; hence the name “high entropy”. This concept was very attractive, in the sense that a single phase cubic alloy with high concentrations showed promise to overcome the strength-ductility trade off; the cubic structure provides multiple available slip systems, promoting ductility, while solid solution strengthening in highly concentrated alloys enhances strength, presumably beyond what is possible by dilute additions. Indeed, a remarkable combination of strength, ductility and fracture toughness was observed in the fcc FeCoCrMnNi, stimulating several subsequent studies on this alloy and its quaternary and ternary derivatives [7, 8].

The significance of configurational entropy on mechanical properties – and consequently the number of components and the equimolar composition – have since been critically questioned [9, 10]. In fact, a new paradigm is being followed, where instead of a search for compositions that favor single phase HEAs, formation of second phases are sought after to take advantage of precipitation hardening [10, 11]. However, the idea of a concentrated solid solution is still attractive, since in addition to the single phase HEAs, the different phases of the newer alloys often comprise of concentrated solid solutions. Therefore, understanding solid solution strengthening mechanisms in concentrated solutions is an important topic, which applies to a wide range of systems beyond HEAs, such as other finite-concentration solid solutions, and Ni- and Co-based superalloys.

Solid solution strengthening stems from the interaction of lattice dislocations with solutes. As a dislocation moves in the crystal, the distortion it induces on the lattice interacts with the distortions around substitutional solutes. Substitutional solutes in cubic materials distort a lattice both geometrically – as a result of size mismatch with atoms of the host lattice – and chemically, by locally introducing a different bonding environment. Consequently, the dislocation/solute interaction energy typically consists of size misfit and more specific chemical core contributions [12–14], where the former results from the interaction of the

volumetric strain field around the solute with the elastic stress field of the dislocation and the latter is caused by the different bonding environment within the nonlinear core and stacking fault regions of the dislocations. The motion of a dislocation is hindered by such interactions, requiring additional resolved shear stress for continued plastic deformation.

Theories of solute strengthening in alloys can be broadly divided into two categories of strong-pinning and weak-pinning models. The strong-pinning models, such as the ones proposed by Friedel [15] and Fleischer [16, 17], treat the solutes as individual point obstacles that pin the dislocations. Dislocation then bows out in the regions between the solutes and can break free from these obstacles upon application of additional stress. On the other hand, the weak-pinning models, originally proposed by Mott [18] and Labusch [19, 20], consider the collective effect of a field of randomly-distributed solutes on the dislocations. Favorable fluctuations in the solute distribution lower the energy of the dislocations, thereby pinning them, and the dislocation bows out between these pinned regions. Under additional resolved shear stress, the dislocations can escape from these obstacles, resulting in increased yield strength. In both strengthening models, the dislocation is treated as an elastic line, and its bow-out has an energetic cost due to the line tension. More recently, Leyson *et al.* [14, 21] proposed a parameter-free Labusch-type strengthening model for dilute alloys. Contrary to the original Labusch's model, it does not postulate any *a priori* interaction range – this typical length scale naturally emerges from the theory – and includes the specific dislocation/solute interaction within the core, that are possibly computed by first principle methods. This model has been successfully applied to predict the solute strengthening of range of fcc [14, 21] and hcp [22, 23] slip and even twinning modes [24], and has shown great agreement with experiments. Moreover, Leyson and Curtin [25] compared the applicability of Friedel vs Labusch-type strengthening models, and concluded that, except for the highly localized dislocation cores, Labusch-type models control the strengthening for concentrations greater than 10^{-4} and temperatures greater than 78K, i.e ranges relevant to most engineering alloys.

The above historical models are developed with the assumption of dilute alloys, where a base element makes the host lattice, and small amounts of alloying elements are introduced as solutes. This assumption is clearly not valid in the case of highly concentrated solid solutions. The contrast is even more pronounced for equiatomic alloys, where the definition of solute and solvent breaks down.

Here we review the solid solution strengthening theories for general random alloys with high elemental concentrations. The initial attempts by Toda-Caraballo *et al.* [26] were based on application of the Labusch model, in its original form, and assuming only elastic misfits contributions to strengthening. The only new theory for solid solution strengthening in concentrated solid solutions, is proposed by Varvenne *et al.* [27]. This theory assumes an effective average medium as the matrix and individual elemental types as solutes interacting with dislocations into the average medium. In the limit of dilute concentrations, this model reduces to the modified Labusch-type model of Leyson *et al.* [14, 21]. We describe this full theory, some numerical validations, useful model simplifications, and some examples of its successful application, in the following section. Other efforts in modeling solute strengthening in HEAs are listed and discussed afterwards. Finally, we conclude by discussing the influence of several materials inputs of existing models as well as future work directions.

EFFECTIVE-MEDIUM-BASED THEORY OF SOLUTE STRENGTHENING

Varvenne *et al.* proposed a theory for predicting the yield strength of random fcc alloys with arbitrary compositions [27]. The theory is based on the assumption that in a general random alloy, each elemental component can be regarded as “solute” in an effective “solvent” representing the average properties of the alloy. The solvent is then formally defined as an effective matrix at the overall average composition (mean field alloy), and solutes correspond to local composition-fluctuation with respect to the overall composition of the effective-matrix reference state [28].

Presentation of the full model

First, the reference material is defined with the average lattice parameter a , elastic constants $\{C_{ij}\}$ and stable and unstable stacking fault energies γ_{SF} and γ_{USF} , all of which correspond to the composition of the random alloy. The usual $\{111\}(110)$ slip systems are considered in this effective fcc matrix, where a (110) type dislocation dissociates onto two Shockley partials, bounding a stacking fault on $\{111\}$ type planes. This setup is shown schematically in Figure 1 taken from Ref. [27].

For an N-component alloy, the interaction energy for a solute of type n at position (x_i, y_j)

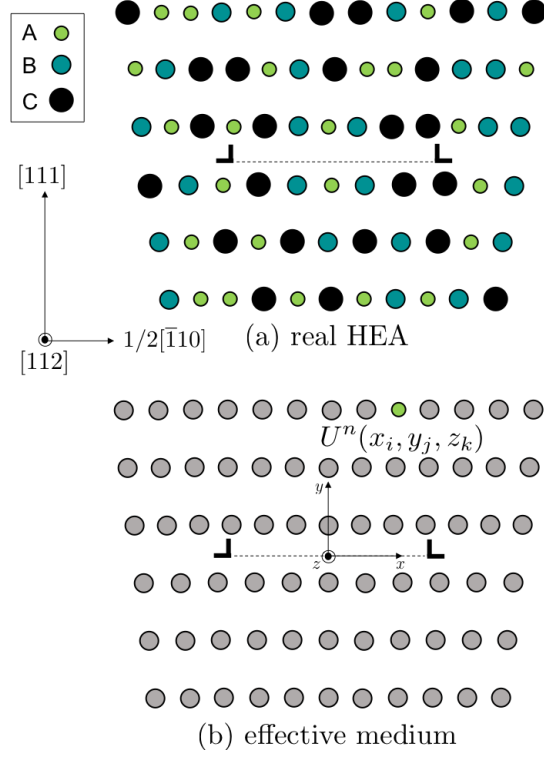


FIG. 1. Effective medium concept for dislocation/solute interactions. (a) shows a random 3-component alloy, with component types A, B and C, containing a dissociated edge dislocation; (b) shows the effective average matrix of the same alloy, with an embedded A “solute” at position (x_i, y_j, z_k) relative to the dislocation centered at the origin, with interaction energy $U^n(x_i, y_j, z_k)$. Adapted from Varvenne *et al.* [27].

from the center of a straight dislocation and at position z_k along the dislocation line is named $U^n(x_i, y_j, z_k)$. Major contributions to this interaction energy are from the elastic interaction of the dislocation’s stress field with the misfit strain tensor of the solute and from the chemical misfit resulting from the change in the bonding environment of the solutes in the partial dislocation core geometry and the stacking fault region between them. In a random solute distribution, local fluctuations in the solute concentrations arise where the dislocation is attracted to the locally favorable fluctuations and is repelled by the unfavorable ones. The dislocation potential energy is lowered by finding the favorable solute fluctuations, requiring higher levels of shear stress to free the dislocation from these obstacles.

An important concept in the theory developed by Varvenne *et al.* is the energy change of a straight segment of dislocation ζ during the glide over a distance w . The relative change

in the position of the dislocation and fixed solutes results in a potential energy change given by

$$\Delta U_{\text{tot}}(\zeta, w) = \sum_{i,j,k,n} s_{ijk}^n [U^n(x_i - w, y_j, z_k) - U^n(x_i, y_j, z_k)], \quad (1)$$

where s_{ijk}^n is an occupancy parameter, which equals 1 if a n-type solute occupies position (x_i, y_j, z_k) and 0 otherwise. The typical favorable fluctuation in the interaction energy – i.e. those that pin the dislocation by lowering its energy – is given by the standard deviation of the *total* potential energy change

$$\sigma_{\Delta U_{\text{tot}}}(\zeta, w) = [\langle \Delta U_{\text{tot}}^2(\zeta, w) \rangle - \langle \Delta U_{\text{tot}}(\zeta, w) \rangle^2]^{1/2}, \quad (2)$$

where the brackets are ensemble averages over the occupancy parameters s_{ijk}^n . This averaging can be performed analytically along the dislocation line segment z_k , neglecting any correlation between the different chemical occupations of atomic sites, which yields

$$\sigma_{\Delta U_{\text{tot}}}(\zeta, w) = \left(\frac{\zeta}{\sqrt{3}b} \right)^{1/2} \Delta \tilde{E}_p(w), \quad (3)$$

where

$$\Delta \tilde{E}_p(w) = \left[\sum_{i,j} c_n ((\bar{U}^n(x_i - w, y_j) - \bar{U}^n(x_i, y_j))^2 + \sigma_{\Delta U_{ij}^n}^2) \right]^{1/2}. \quad (4)$$

In the above equation, $\bar{U}^n(x_i - w, y_j)$ is the average value of $U^n(x_i, y_j, z_k)$ over the sites along the dislocation line z_k at in plane position (x_i, y_j) , and $\sigma_{\Delta U_{ij}^n}^2$ is the associated standard deviation.

While a straight segment of dislocation L reduces its energy by bowing towards the favorable solute interactions, the increase in dislocation line – from straight to wavy configurations – costs energy due to the line tension.

Figure 2 shows the schematic of the original straight dislocation of length L adopting a wavy configuration consisting of straight segments of length 2ζ and of amplitude w as it moves through the random field of solutes. The total energy change corresponding to this event is given by, assuming $w \ll \zeta$

$$\Delta E_{\text{tot}}(\zeta, w) = \Delta E_{LT}(\zeta, w) - \sigma_{\Delta U_{\text{tot}}}(\zeta, w) \left(\frac{L}{2\zeta} \right) = \left[\Gamma \frac{w^2}{2\zeta} - \left(\frac{\zeta}{\sqrt{3}b} \right)^{1/2} \Delta \tilde{E}_p(w) \right] \left(\frac{L}{2\zeta} \right), \quad (5)$$

where Γ is the dislocation line tension. The pinned dislocation geometry is obtained by minimizing the total energy change with respect to both the segment length ζ and the

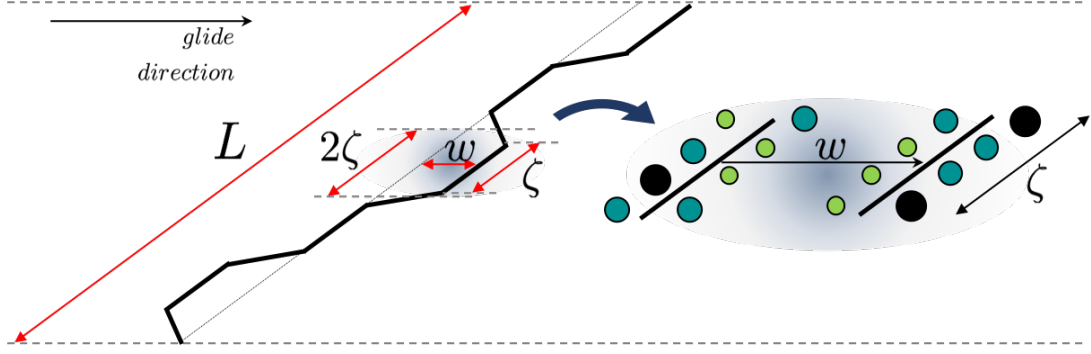


FIG. 2. Schematic of a straight dislocation segment of length L , adopting a low-energy wavy configuration as it moves through the random field of solutes. The configuration consists of segments of length 2ζ with amplitude w . The total dislocation energy is optimized with respect to both ζ and w to obtain the critical lengths ζ_c and w_c . Adapted from Varvenne *et al.* [27].

amplitude w . The critical segment length ζ_c is

$$\zeta_c(w) = \left(4\sqrt{3} \frac{\Gamma^2 w^4 b}{\Delta \tilde{E}_p^2(w)} \right)^{1/3}. \quad (6)$$

The subsequent optimization with respect to w needs to be done numerically to obtain the critical amplitude w_c . In fact, multiple minima – i.e. multiple pairs of $(\zeta(w_c), w_c)$ values – can be found [22, 27, 29, 30], especially when there exist a large dissociation between the partial dislocations, like in HEAs. This is further elaborated in the discussion section.

In the minimum energy configuration, segments of ζ_c sit in a local potential energy well. Approximating this energy well with a sinusoidal function gives the total energy barrier as $\Delta E_b = 1.22 \left(\frac{w_c^2 \Gamma \Delta \tilde{E}_p^2(w_c)}{b} \right)$ for the dislocation to escape the energy well, i.e to unpin. The dislocation overcomes this barrier through a thermally activated process, assisted by an applied resolved shear stress. The zero temperature flow stress required to overcome ΔE_b is then

$$\tau_{y0} = \frac{\pi}{2} \frac{\Delta E_b}{b \zeta_c(w_c) w_c} = 1.01 \left(\frac{\Delta \tilde{E}_p^4(w_c)}{\Gamma b^5 w_c^5} \right)^{1/3}. \quad (7)$$

At finite temperature, the energy barrier can be overcome with lower stress levels $\tau_y(T, \dot{\epsilon})$ as

$$\tau_y(T, \dot{\epsilon}) = \tau_{y0} \left[1 - \left(\frac{kT}{\Delta E_b} \ln \frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right)^{2/3} \right], \quad (8)$$

where $\dot{\epsilon}$ is the plastic strain rate and $\dot{\epsilon}_0$ is a reference strain rate value obtained from the

dislocation density, Burgers vector, typical slip distance and attempt frequencies from the Orowan relationship [14, 27].

At higher temperature/lower stress regimes [14, 29, 31] the flow stress is better represented by

$$\tau_y(T, \dot{\epsilon}) = \tau_{y0} \exp\left(-\frac{1}{0.51} \frac{kT}{\Delta E_b} \ln \frac{\dot{\epsilon}_0}{\dot{\epsilon}}\right). \quad (9)$$

In the dilute alloy limit, the present theory is equivalent to the previous predictive model of Leyson *et al.* [14, 21, 22, 30]. The inputs to the generalized parameter-free model are the Burgers vector b , the dislocation line tension Γ , and the various $\{U^n(x_i, y_j, z_k)\}$, i.e. the interaction energies of the various “solutes” with the dislocation. All these quantities are evaluated with respect to the effective-medium reference state. To validate some aspects of this model, Varvenne *et al.* [27] compared direct molecular statics simulations of the flow stress of short dislocation segments in a series of model $(\text{FeNi})_{1-x}\text{Cr}_x$ alloys to the theory predictions, with all inputs computed from atomistics (using an EAM potential [32]). Note that with these short segments, the dislocations remain straight under applied stress in molecular simulations, and thus model predictions are made without the line tension contribution. A good agreement was obtained for the different investigated alloys, thus validating the simplified description of the potential energy landscape, and the internal length scales controlling the materials strength.

Considering real alloy systems, in the dilute limit, and assuming solutes do not alter the core geometry of the dislocation, the key interaction energies can be computed via direct first principles calculations of the dislocation [13, 23, 33, 34]. However, in HEAs, modeling the dislocation core with first principles calculations is very difficult, in particular due to large simulation sizes necessary to capture chemistry changes along the dislocation line (see discussion section).

Model simplification using elasticity

Alternatively, the dislocation/solute interaction energy can be approximated by a combination of size misfit – interaction of the solute misfit volume with the pressure field of the dislocation – and of chemical misfit – interaction of the solute with stacking faults as a surrogate for the dislocation core – contributions to the interaction energy [30, 35]. Beyond the dilute limit, calculations of the size and stacking fault misfit parameters are still challenging

and require several simulations of sufficient size and accuracy to capture the fluctuations from the average values caused by high concentrations of multiple elements [36]. In light of these complications, Varvenne *et al.* [27] presented a reduced version of their theory of strengthening to consider only the main elasticity, i.e the size misfit, contribution to the interaction energy. This interaction energy is a result of the work done by the pressure field of the dislocation $p(x_i, y_j)$ on the misfit strain created by inserting an atom of a different size in the host lattice, and is given by

$$U_{el}^n(x_i, y_j, z_k) = -p(x_i, y_j)\Delta V_n(x_i, y_j, z_k), \quad (10)$$

where $\Delta V_n(x_i, y_j, z_k)$ is the change in total volume of the average medium as a solute of type n is inserted at position (x_i, y_j, z_k) .

Representing the dislocation pressure field with $p(x_i, y_j) = -\frac{\mu(1+\nu)}{3\pi(1-\nu)}f(x_i, y_j)$, where $f(x_i, y_j)$ is a dimensionless pressure field from a distribution of normalized Burgers vectors on the glide plane and μ and ν are the elastic constants, and substituting Equation 10 into Equation 4 results in

$$\Delta \tilde{E}_p(w) = \frac{\mu(1+\nu)}{3\pi(1-\nu)} \left[\sum_{ij} \Delta f_{ij}^2(w) \right]^{1/2} \times \left[\sum_n c_n \left(\Delta \bar{V}_n^2 + \sigma_{\Delta V_n}^2 \right) \right]^{1/2}. \quad (11)$$

In the above equation $\Delta f_{ij}(w) = f(x_i - w, y_j) - f(x_i, y_j)$. The term $\sum_n c_n \left(\Delta \bar{V}_n^2 + \sigma_{\Delta V_n}^2 \right)$ emerges as the main misfit volume quantity, in which $\Delta \bar{V}_n$ is the average misfit volume of solute n and $\sigma_{\Delta V_n}$ is the standard deviation. Following the procedure in Equations 5-7 yields τ_{y0} and ΔE_b as

$$\tau_{y0} = 0.051\alpha^{-1/3}\mu \left(\frac{1+\nu}{1-\nu} \right)^{4/3} f_1(w_c) \times \left[\frac{\sum_n c_n \left(\Delta \bar{V}_n^2 + \sigma_{\Delta V_n}^2 \right)}{b^6} \right]^{2/3}, \quad (12)$$

$$\Delta E_b = 0.274\alpha^{1/3}\mu b^3 \left(\frac{1+\nu}{1-\nu} \right) f_2(w_c) \times \left[\frac{\sum_n c_n \left(\Delta \bar{V}_n^2 + \sigma_{\Delta V_n}^2 \right)}{b^6} \right]^{1/3}. \quad (13)$$

Here, $f_1(w_c) = \left[\left(\frac{b}{w_c} \right)^{5/2} \sum_{i,j} \Delta f_{ij}^2(w_c) \right]^{2/3}$ and $f_2(w_c) = \left[\left(\frac{w_c}{b} \right)^2 \sum_{i,j} \Delta f_{ij}^2(w_c) \right]^{1/3}$ are the minimized dislocation core coefficients, and the line tension is approximated by the elasticity relation $\Gamma = \alpha\mu b^2$, where $\alpha = 0.123$ is a dimensionless number rescaled from direct atomistic simulations [27].

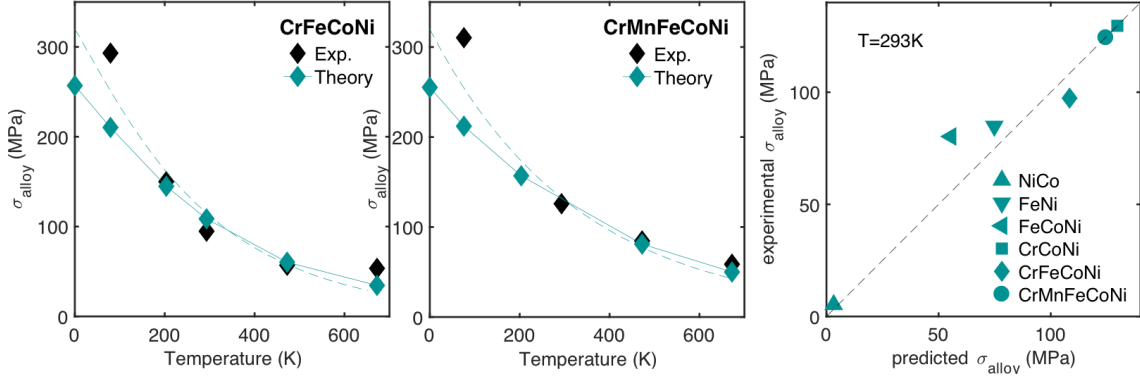


FIG. 3. Comparison between experimental and theoretical prediction of strength. Yield stress vs. temperature are shown for (a) CrFeCoNi and (b) MnCrFeCoNi equiatomic alloys [37, 38], as measured (black symbols) after subtraction of the Hall-Petch contribution to strength and as predicted by the theory (blue symbols) Adapted from Varvenne *et al.* [27]. Theoretical predictions of flow stress are converted into uniaxial yield strengths $\sigma_y(T, \dot{\epsilon})$ by applying the Taylor factor of 3.06.

The elasticity-based reduced version of the theory is fully analytic and easily transferable to any new alloy system: the only inputs to this model are elastic constants, lattice parameters, dislocation core structure, and accurate solute misfit volumes, at the targeted composition. These parameters are either fairly computable by atomistic simulations or can be extracted/evaluated from experiments.

Comparison with experiments

Varvenne *et al.* [27] first applied the reduced theory to predict the strength of NiCoCrFeMn high entropy alloy and some of its derivatives, using only experimental information. In particular, the average misfit volumes $\Delta\bar{V}_n$ are obtained from experimentally measured atomic volumes in various alloys from this family and application of the Vegard’s law.

Figure 3 shows the comparison between theory and experiments in predicting the strength of a set of equiatomic alloys from the NiCoCrFeMn. The agreement is generally great, particularly at moderate temperatures, given the approximations in the reduced version of the model. At T=77 K, the theory underestimates strength. The authors attribute this to a possible combination of (i) line tension effect – not precisely known – which influence

is examined in the discussion section, (ii) need for more accurate calculations of misfit volumes, dislocation core structures and interaction energies with solutes (for example via direct first principles calculations), and (iii) potential Å-scale fluctuations, which are not captured in the model, and could become dominant at very low temperatures. The overall agreement highlights the robustness of the reduced model, in the sense that it takes only a few simple quantities as inputs, and without any adjustable parameters, predicts strength in very good agreement with experiments. Later, Varvenne and Curtin applied this model to CoCrFeNiAl_x and CoCrFeNiMnAl_x family of alloys [39], and to the PdPtRhIrCuNi Noble Metal HEA [40], with similarly good agreement with experimental predictions.

More recently, Laplanche *et al.* measured the activation volumes of plastic flow in CrMnFeCoNi alloy to identify the operative deformation mechanisms [41]. Activation volume corresponds to the volume of the material that is involved in a thermally activated process under the resolved shear stress τ at a certain temperature and is given by

$$V = - \left. \frac{\partial \Delta G(\tau)}{\partial \tau} \right|_T ,$$

where $\Delta G(\tau)$ is the stress-dependent Gibbs free energy corresponding to the gliding dislocation overcoming various obstacles (eg. solute atoms, precipitates, forest dislocations). The activation volumes range from the order of b^3 (where b is the magnitude of the Burgers vector) for individual point defects to $\approx 1000b^3$ for collective solute fluctuations in dilute alloys. Therefore, measuring activation volumes reveals the intrinsic length scales involved in the thermally activated processes of plasticity, thereby providing insight into the operative deformation mechanisms. Measurements of activation volumes in the CrMnFeCoNi showed that the plastic flow in this alloy is governed by a combination of (i) rate-independent Hall-Petch strengthening (ii) thermally activated solute strengthening and (iii) forest hardening; a behavior typical of other usual FCC alloys. In particular, the thermally-activated solid solution strengthening component was compared to the theoretical predictions of activation volume by the model of Varvenne *et al.* The agreement between theoretical and experimental activation volumes is comparable to the one achieved for dilute alloys [14], showing that the effective-medium theory captures the essential concept of solute strengthening in these alloys and consequently, the compositional complexity of this alloy does not induce any new strengthening mechanism.

OTHER MODELING APPROACHES

One of the first attempts to model solute strengthening in HEAs was made by Toda-Caraballo and Rivera [26]. The authors start from the original Labusch's approach and consider its extension to dilute multi-component solid solutions [19, 42]. The zero-temperature solute strengthening is expressed there as

$$\Delta\tau_{ss} = \left[\sum_n B_n^{3/2} c_n \right]^{2/3}, \quad (14)$$

where c_n is the concentration of solute n , B_n is the hardening parameter defined as

$$B_n = 3\mu\epsilon_n^{4/3}Z_0; \quad \epsilon_n = \left(\eta_n'^2 + \alpha_0^2\delta_n^2 \right)^{1/2}, \quad (15)$$

where μ is the shear modulus of the alloy, ϵ_n a mismatch parameter and Z_0 a fitting constant, i.e. an *adjustable* parameter. ϵ_n incorporates the modulus and size misfits η_n' and δ_n as

$$\eta_n' = \frac{\eta_n}{1 + 0.5|\eta_n|}; \quad \eta_n = \frac{1}{\mu} \frac{d\mu}{dc_n}; \quad \delta_n = \frac{1}{a} \frac{da}{dc_n}, \quad (16)$$

where a is the lattice parameter of the alloy and α_0 is an *empirical* parameter that differentiates between edge and screw dislocation interactions with solutes. The adaptation to HEAs proposed by Toda-Caraballo and Rivera consists in redefining the modulus and size misfits for high concentration materials, actually making an implicit effective medium assumption as all quantities are defined with respect to the average HEA composition. The temperature-dependence of the strength is then introduced with a functional form analogous to Eq. 9, with an energy barrier taken as a constant dependent on the material. Assuming then Vegard's law for the lattice constant and linear variation of shear modulus with composition, misfit parameters and consequently the hardening parameters for the HEAs were calculated and compared with experimental values, and good qualitative agreements were achieved. In particular, the dominant role of the elastic size misfit in FCC materials was identified.

To make connection with the effective medium model presented in the previous section, we proceed from the reduced elasticity version of Eq 12, neglecting the misfit volume standard deviation terms. Then, Eq. 12 for the zero-temperature can be matched to Eq. 14 by imposing $B_n = 0.051\alpha^{-1/3}f_1(w_c) \left(\frac{1+\nu}{1-\nu} \right) \mu \left(\frac{\Delta V_n}{b^3} \right)^{4/3}$, to be compared with $B_n = 3\alpha_0^{4/3}Z_0\mu\delta_n^{4/3}$

when the modulus misfit is neglected. Both approaches are thus similar, showing the importance of the HEA shear modulus and of the size misfit quantity. However the derivation by Varvenne *et al.* includes additional material inputs (dislocation core structure, line tension, etc.) - that are embedded into an adjustable parameter by Toda-Caraballo and Rivera - and the full version of the theory includes the solute/dislocation interactions, computable from atomistic simulations, and thus going beyond the elasticity assumptions. In particular, ignoring the details of the core structure and of the energy barrier variation with composition and material quantities, Toda-Caraballo and Rivera’s model will not be able to predict the high-temperature strengthening regime that as been discussed elsewhere [27, 29, 30] (see also the discussion section).

More recently, Walbrühl *et al.* [43] proposed an Integrated Computational Materials Engineering (ICME) approach to model solid solution strengthening in multicomponent alloys. Their perspective is much more pragmatic, and stems from the difficulty to compute the material inputs for a high number of systems in physically-based models. Instead, they follow an empirical approach, still using the Labusch’s $c_n^{2/3}$ dependence of the strength – where c_n is again the concentration of element n – but considering a nonlinear composition dependence of the strengthening parameters that are globally fitted in order to directly reproduce the hardness of a database of 895 alloys from the literature. The adopted functional forms are not physically derived, but are meant to account for both substitutional and interstitial solute strengthening and includes the presence of various phases. The solute strengthening part of the yield strength is converted into hardness by applying a constant factor for all materials. After an adjustment procedure, they provide a database of parameters for predicting strengthening in a wide range of multicomponent alloys.

While the authors recognize the lack of physical basis / derivation of their model, they assign the adjustable parameters to various physical mechanisms, i.e. Peierls-like resistance and solute strengthening (the latter embeds both solute and precipitate strengthening in their model). Incidentally they attempt to draw physical conclusions, e.g. in the CoCrFeNiMn HEA, where only half of the strength would be due to solid strengthening, whereas Peierls stress is almost null in FCC materials, as already shown numerically for random multicomponent alloys [28]. This should be proscribed in a fully empirical approach. Next, the agreement between the fitted model and the experimental data for the hardness is within 13%, a quite large deviation for a data interpolation. Part of this is due to uncertainties in

experimental measurements, and to the uncontrolled Hall-Petch effect, as the grain size is often not reported in the experimental hardness database, even if its impact on the strength can be important [37, 38]. Finally, the transferability of this model to other alloy systems is not ensured, which is a general issue of fitting approaches that require recalibration of the model parameters for investigation of new materials. And the transferability could possibly be lowered by the identified issues on the adjustment hardness database. Consequently, if one is keen on getting pragmatic, adopting machine learning / deep learning approaches, completely leaving physical arguments, and having much flexible functional forms and number of parameters, would be even more appropriate for material design.

DISCUSSION

In this section, the effective-medium theory of strengthening for random alloys, providing a firm theoretical foundation for the observed strengthening trends without any adjustable parameter, is used to discuss the influence of several material inputs, and how they could be computed for specific materials. All along the discussion, we highlight remaining issues and challenges for future work in the area.

Importance of the line tension

While a useful concept to describe the elastic energy cost of a dislocation bow-out [15, 19, 21, 27, 44, 45], the line tension is not an easy quantity to estimate for a given material. It depends on the dislocation length, dislocation character, dislocation core, and on the anisotropy of the matrix material [46–48]. The most common assumption in both historical and more recent models is to assume a unique and fixed value per studied material for the line tension, and to assume isotropic elasticity. In Ref. [27], a rescaling $\Gamma = \alpha\mu b^2$ was proposed, with $\alpha = 0.123$ estimated for edge dislocations by comparison with direct line tension measurements in atomistic simulations, performed on a FeNiCr equiatomic alloy, using an EAM potential [32]. This approach presents the advantage of an easy estimate of Γ for any new material of interest.

The importance of such simplifications can be examined through a sensitivity analysis. A representative example is shown in Fig. 3a (dashed lines), where the strength is predicted

with Γ values either twice or half the rescaled value using $\alpha = 0.123$. Strengths at intermediate temperatures are only weakly dependent on Γ , while below $T = 77K$, the effect of Γ becomes more visible. This can be rationalized by computing the first derivative of strength with respect to the line tension as $\partial\tau_y(T)/\partial\Gamma = -\tau_y(T)/3\Gamma$, using Eq.9, and noting that $\tau_{y0} \propto \Gamma^{-1/3}$ and $\Delta E_b \propto \Gamma^{1/3}$. Thus, at intermediate temperatures, when doubling Γ , the effect on τ_{y0} will be partially compensated by the effect on ΔE_b , and the strength will not be modified. On the other hand, for $T \rightarrow 0$, $\partial\tau_y(T)/\partial\Gamma \simeq -\tau_{y0}/3\Gamma \propto \Gamma^{-4/3}$ and then doubling Γ will have much impact on the strength. Consequently, refined line tension measurements would be worth only for the prediction of very low-temperature strengths. Note that similar sensitivity to Γ has been observed [41] for activation volumes due to solute strengthening.

Nevertheless, a detailed methodological work, going beyond this simple analysis, and with a proper investigation of the effect of the dislocation length [30] and elastic anisotropy on the line tension, and thus the predicted alloy solute strengthening quantities, remains to be done.

Role of the dislocation core structure

Accurate knowledge or modeling of the dislocation core structure is usually important for plasticity [49], and in particular has been underlined in the context of solute strengthening in dilute alloys, by various authors [13, 14, 21, 25, 45, 50, 51]. This motivated first-principles computations of the dislocation core structures in the pure elemental materials of interest, or of the less cumbersome generalized stacking fault energy (GSFE) maps, that can be used as inputs to Peierls-Nabarro models so as to obtain the dislocation core structure.

In HEAs or any concentrated solid solution alloy, the core structure also matters for the strength; this appears in the reduced elasticity model of Eq. 10 for the solute / dislocation interaction, and Eqs. 12 and 13 for the strength. The core structure determines the dislocation pressure field, and then the characteristic lengths ($\zeta(w_c), w_c$) and the minimized core coefficients $f_1(w_c)$ and $f_2(w_c)$ of τ_{y0} and ΔE_b , respectively. Its influence on the strength is then analyzed through a parametric study, with the Burgers vector distribution of the FCC edge dislocation modeled by a double gaussian function $\frac{db}{dx} \sim e^{-\frac{1}{2}\left(\frac{x-d/2}{\sigma}\right)^2} + e^{-\frac{1}{2}\left(\frac{x+d/2}{\sigma}\right)^2}$, with d the splitting distance between the partial Shockley dislocations, and σ the partial spreading, and using isotropic elasticity to compute the dislocation pressure field. The com-

puted minimized core coefficients versus d , and for $\sigma = 1.5b$, are displayed in Fig. 4a and b. For sufficiently large d values (typically $d > 10b$), there exist two minimum energy configurations leading to two different minimized core coefficients for both τ_{y0} and ΔE_b . The first minimized core coefficients $f_1(w_{c1})$ and $f_2(w_{c1})$ are associated with the high stress / low-temperature regime, and are insensitive to d , that is related to the stable stacking fault energy (SFE) as $d = \mu b(2 + \nu)/(24\pi(1 - \nu)\gamma_{\text{SF}})$, following an isotropic elasticity model. The second minimum energy configuration corresponds to a larger w_c value, and is active at a lower stress / higher temperature regime. It is associated with a high energy barrier – typically 3-5 eV – which thus provides a high temperature plateau stress whose value is much more sensitive to d and thus to γ_{SF} . The effect of the partial spreading is finally investigated by comparing the core coefficient values for the first minimum, obtained with $\sigma = 1, 1.5$, and $2b$ (Fig.4). The $f_1(w_{c1})$ and $f_2(w_{c1})$ values for large d are entirely fixed by σ , a value roughly scaling with the inverse of the unstable stacking fault energy (USFE), $\sigma \sim \gamma_{\text{USF}}$ [52]; accurate estimate of σ would be required. For smaller separation distances, d and σ both induce variations in $f_1(w_c)$ and $f_2(w_c)$, meaning that in these cases the knowledge of both SFE and USFE is important for the strength.

Discussing now specifically the case of HEAs, both experiments and *ab initio* calculations estimated low γ_{SF} / large d values [53–55] for the Co-Cr-Fe-Ni-Mn class of HEAs, suggesting that the exact knowledge of d would not be necessary for HEA strength at low to intermediate temperature. Concerning σ , a value of $1.5b$ was proposed [27] as a typical value resulting from atomistic simulations of model EAM HEAs and various elemental alloys, and provided good agreement with experimental strengths [27, 39, 40]. However, any systematic and intensive investigation of GSFE curves versus HEA composition coupled to Peierls-Nabarro modeling of the core, aiming at (i) establishing if large d is a generic behavior in HEAs and (ii) understanding the effect of partial core spreading on the strength, would be beneficial to the community.

The role of the dislocation core structure has been discussed here within with the assumption of isotropic elasticity for the dislocation pressure field, whereas many alloys are elastically anisotropic. A more detailed analysis, accounting for the elastic anisotropy of the HEAs, would be an interesting direction for future work.

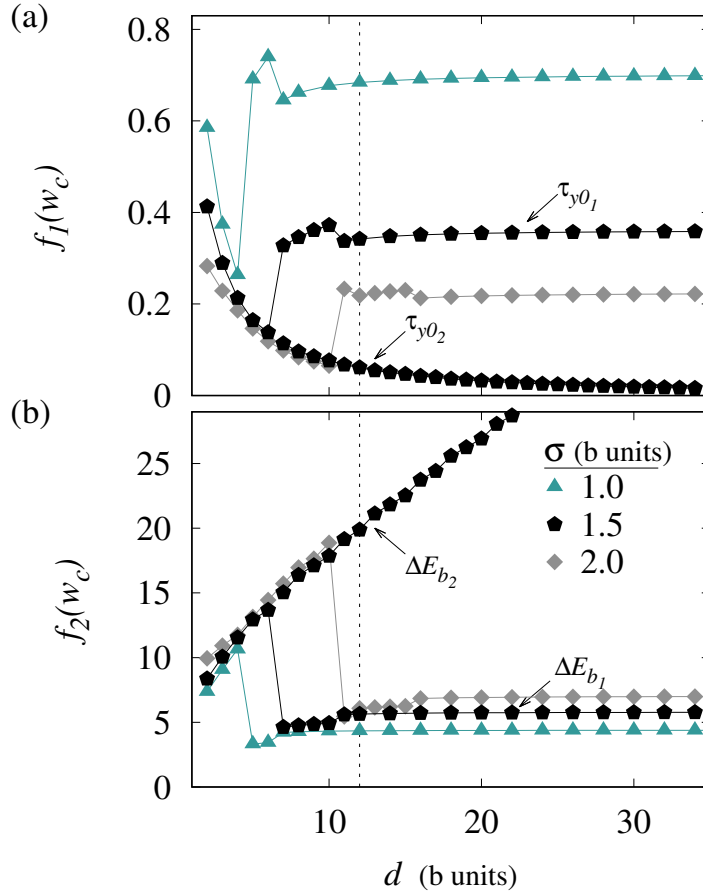


FIG. 4. Influence of the dislocation core structure on the minimized core coefficients (a) $f_1(w_c)$ and (b) $f_2(w_c)$, appearing in Eqs. 12 and 13 for τ_{y0} and ΔE_b , respectively. See main text for details.

Difficulties for DFT computation of model inputs

Introduction of HEAs, where the notion of solute and solvents is to be revisited, stimulated the need to rethink the solute strengthening models. The available physically-based models take as inputs, in the more general version, precise dislocation core geometry, solute/dislocation interaction energies and the dislocation line tension, preferably directly computed with first principles calculations. Such direct calculations are currently prohibitive in case of HEAs; the elasticity reduction of the model, with simplified inputs (Burgers vector, elastic constants, stable and unstable stacking faults, and misfit volumes), is thus valuable and has been shown to capture the main contributions to strengthening, as validated by experiments. The state-of-the art techniques to account for chemical disorder, i.e. the su-

percell approach coupled to the concept of special quasi-random structures (SQS) [56, 57], or the approach based on the coherent potential approximation (CPA) [58–61], allow to compute these materials quantities, with some care. Using the first approach, large simulations sizes and / or several simulations are necessary to capture the reliable statistics of the “average” response of the alloy and the local fluctuations, causing deviations from the average behavior. This has been demonstrated in the simpler case of stacking fault calculations in Refs [55, 62]. Alternatively, the second approach reproduces a perfectly disordered state very efficiently, but is unable to include the local lattice distortions, which importance depends on the computed quantity. As a consequence, both approaches remain competitive. Currently, first principles values of b , C_{ij} , γ_{SF} and γ_{USF} have been reported for several HEAs, as nicely summarized in Ref. [36]. Misfit volume values are less common; a few computations of average bond lengths, bond length fluctuations and elastic size misfit can be found [63, 64].

Note finally that any progress in more detailed calculations of solute/dislocation interaction energy and dislocation core structure should make the strengthening predictions even more robust.

Short range ordering

An important assumption in all previously discussed strengthening models is a random distribution of atoms in the alloy. This is certainly a good approximation for dilute alloys as well as several HEA systems that are shown to be random experimentally [37, 39, 41, 65], likely due to the so-called “sluggish diffusion” effect in HEAs. However, short range ordering (SRO), i.e. correlation at small distances between chemical occupations of the atomic positions in the alloy, is thermodynamically expected when approaching transition temperatures. Such SRO arises from interactions between alloy elements, and has been experimentally observed or theoretically predicted for some multicomponent alloys [66–70]. In dilute alloys, the effect of SRO on strengthening has been historically envisioned through the formation of pairs, triplets or clusters, due to solute/solute interactions. Those clusters are then considered as new, independant and randomly distributed species interacting with the dislocation, and applying conservation laws their contribution to strengthening can be included in the framework of the standard strengthening models. Either additional strengthening or softening as compared to equivalent solid solutions having only isolated solutes is then observed

[42, 71]. SRO also modifies the statistics of dislocation/solute and solute/solute interactions (cf Eq. 4); this would be possible to include in the Labusch-type models but would likely lead to a loss of analyticity in the equations. In HEA systems, the effect of SRO could be included in the generalized theory presented here, with a more comprehensive energetic model and appropriate treatment of statistics, and re-defining the notion of clusters, similarly to what has been done for solutes in random concentrated alloys. The details of addition of SRO effect and an assessment of its relevance to total strengthening, particularly at finite temperatures, remains a challenging task.

Conclusion

The Labusch-type models combined with an effective-medium approach work well in HEA systems with low Peierls barrier, such as FCC alloys. In materials such as BCC alloys the generally accepted deformation mechanism is kink-pair nucleation for screw dislocation motion. Depending on the effect of solutes on this process, solutes can soften as well as strengthen the dislocation motion [72, 73]. Therefore, solution strengthening/softening of BCC high entropy alloys await for (i) identification of the relevant operating mechanisms and (ii) for the development of a related mechanistic theory, dealing with arbitrary compositions.

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