Stability maps to predict anomalous ductility in B2 materials

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Stability maps to predict anomalous ductility in B2 materials

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While most B2 materials are brittle, a new class of B2 (rare-earth) intermetallic compounds is observed to have large ductility. We analytically derive a necessary condition for ductility (dislocation motion) involving (111) versus (001) slip and the relative stability of various planar defects that must form. We present a sufficient condition for antiphase boundary bistability on [110] and [112] planes that allows multiple slip systems. From these energy-based criteria, we construct two stability maps for B2 ductility that use only dimensionless ratios of elastic constants and defect energies, calculated via density functional theory. These two conditions fully explain and predict enhanced ductility (or lack thereof) for B2 systems. In the 23 systems studied, the ductility of YAg, ScAg, ScAu, and ScPd, ductile-to-brittle crossover for other rare-earth B2 compounds, and brittleness of all classic B2 alloys and ionic compounds are correctly predicted.

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I. INTRODUCTION

In 2003, Gschneidner et al. discovered a family of ductile rare-earth/transition-metal (RM) intermetallic compounds with the body-centered-cubic-based B2 (or CsCl) crystal structure.1 The current list of known ductile B2 compounds can be found in Ref. 2. In contrast to the brittleness of classic B2 alloys, the ductility of YAg is comparable to face-centered-cubic Al, and YCu is half that of YAg. As line compounds are usually brittle,3 the reason for anomalous ductility in RM compounds remains open. Moreover, some RM compounds, such as (Tb0.88Dy0.12)Zn (Ref. 4) and YMg,5 are brittle. Hence, the questions: Why are they different? Can anomalous ductility be predicted on a system-dependent basis?

Much work has been done in determining the dominant slip systems of the B2 alloys. As discussed in the review articles by Yamaguchi and Umakoshi6 and Baker,7 (111) and (001) are the two main observed slip directions for dislocation motion in B2 materials (Fig. 1). Yet no previous theories have attempted to predict B2 ductility because all the known alloys and ionic compounds are brittle. For example, polycrystalline NiAl has only a 2% elongation upon fracture.8 Baker concluded that limited ductility is associated with (001) slip, and brittleness with (111) slip.9 While off-stoichiometric B2 alloys exhibit improved ductility, yield strength is sacrificed, which is not useful for practical purposes.3 In contrast to B2 alloys, this new class of RM compounds has an exact stoichiometry, and the compounds are nearly elastically isotropic.1

Following the discovery of the RM compounds, there have been several experimental10–12 and theoretical13,14 studies. Morris et al. have hypothesized that the enhanced ductility in the Y-based compounds is due to the competing structural stability of B33 and B27 phases, obtained by introducing a periodic array of (001) {110} superintrinsic stacking faults (SISFs) to the B2 lattice.12 However, the fact that not all the RM-B2 compounds are ductile highlights the complications with classification of the slip modes and the prediction of their ductility. More recently, Gschneidner et al. established a correlation between the absence of d electrons and measured ductility.3 However, a direct explanation from the perspective of ductility involving dislocation motion and defect energetics is lacking. Such a theory permits prediction, as well as correlations to specific electronic features, to be made, while relating observed ductility measures to features in the electronic structure is fruitful but not a theory.

To address the atypical ductility possessed by some RM compounds and the unresolved issue of predicting (111) versus (001) slip, we provide a quantitative explanation from mesoscale dislocation mechanics using energy-based stability criteria, whose parameters can be calculated from density functional theory (DFT). In short, we present a predictive theory for ductility in ideal B2 compounds. From stability criteria derived for the B2 structure, we provide a necessary and sufficient condition for increased ductility in B2 systems, which are displayed in terms of predictive dimensionless maps. We apply these maps to three types of B2 materials: (1) Y-based and Sc-based compounds (YAg, YCu, YIn, YRh, YMg, YZn, ScAg, ScAu, ScCu, ScPd, ScPt, ScRh, and ScRu), (2) classic alloys (NiAl, FeAl, AuCd, AuZn, CuZn, and AgMg), and (3) ionic compounds (CsCl, CsI, TlBr, and TlCl). Any proposed B2 compound can be added to the map to predict its relative ductility. The possibilities can be narrowed using only the Zener anisotropy ratio.

II. BACKGROUND

For dislocation-mediated deformation, both elastic anisotropy and planar defect energies (e.g., antiphase boundaries $\gamma_{\text{APB}}^{hkl}$ or stacking faults $\gamma_{\text{SF}}^{hkl}$) in the competing Miller-indexed (hkl) slip planes are relevant. Clearly, the more elastically isotropic a system, the easier for dislocation movement to other slip planes under shear. As noted, the new ductile B2 systems are nearly elastically isotropic,1 with Zener anisotropy ratio $A$ close to 1, where

$$A = \frac{2c_{44}}{c_{11} - c_{12}}.$$ (1)
Here, the \( c_{ij} \)'s are the cubic elastic constants, and, in particular, \( c_{44} \) is the shear modulus. For a B2 lattice constant of \( a \), the product of \( c_{44}a \) has units of \( \gamma \) (in \( \text{mJ/m}^2 \)). For an energy-based criterion for ductility under shear, dimensionless ratios are relevant, reflecting relative energies; two ratios associated with the energetics of slip directions and defect formation, making the simple maps, are

\[
C = \frac{\gamma_{\text{APB}}}{\gamma_{\text{SF}}} \frac{1}{c_{44}a}, \quad (2)
\]

\[
\delta = \frac{\gamma_{\text{SF}}}{\gamma_{\text{APB}}} \gamma_{\text{APB}}, \quad (3)
\]

These quantities can be obtained via DFT calculations.

In a recent study of the L1_2 binaries and pseudobinaries, the occurrence/loss of the yield-stress anomaly was predicted in all systems studied by considering the necessary condition for the stability of APB versus SISF and a sufficient condition for the stability of APB(111) versus (100) for cross-slip of screw dislocation segments. The APB and SISF energies, as well as \( c_{ij} \), were obtained using DFT. The necessary and sufficient conditions were derived, respectively, by Paidar, Pope, and Yamaguchi (modified by Liu et al.) and Saada and Veyssiere. The resulting stability map is applicable to any L1_2 material. Here, we adopt a similar approach. We construct two maps based on energy-stability criteria for competing slip modes in B2 structures that fully explain and predict enhanced ductility (or lack thereof) in B2 systems.

### III. METHODS

DFT calculations were performed to obtain required parameters of the theory. We employed the Vienna Ab Initio Simulation Package (VASP) that uses pseudopotentials with a projector augmented wave (PAW) basis. We adopted the generalized gradient approximation (GGA) to the exchange-correlation functional. The lattice \( a \) and elastic \( c_{ij} \) constants were calculated for two-atom B2 cells with 20 \( \times \) 20 \( \times \) 20 \( \mathbf{k} \)-point meshes. Total energies (forces) were converged below 0.1 meV/cell (1 meV/Å). Due to errors in GGA functionals, \( a \) for metals are overestimated, which affect the values \( c_{ij} \) and \( \gamma \) because the defect planes are farther apart and lowers the defect energy, giving material-dependent errors. Therefore, we used \( a_{\text{expt}} \) (if known) to create the maps to remove nonsystematic errors from calculated quantities. (The value of \( a_{\text{expt}} \) is unknown for YIn.) Note that removing such nonsystematic error is critical for predicting quantitatively other deformation processes, such as twinning, because the atomic planes away from the planar defects are separated by geometric multiples of \( a_{\text{expt}} \) (the same distances as in experiment), but relaxation around the defects plane is included, so DFT provides a more correct shear surface energy.

The planar defect energies of APB(110) and SF(110) were calculated for 32-atom unit cells having at least 12 \( \times \) 12 \( \times \) 2 \( \mathbf{k} \) points. The APB(112) was calculated using a 24-atom unit cell and 8 \( \times \) 8 \( \times \) 4 \( \mathbf{k} \) points. Examples of the various unit cells are shown in Fig. 2. The \( \mathbf{k} \)-point meshes were chosen such that the reciprocal axes had a similar density of \( \mathbf{k} \) points. The aspect ratio in \( \mathbf{k} \) space, then, was roughly the reciprocal of that in real space. APBs and SFs on the \( \{110\} \) plane were separated by...
eight layers of atoms, whereas APB\{112\}‘s were separated by six layers. To remove errors for \(k\)-point meshes, the perfect cell had the same number of atoms and cell shape as the defective cell. (Note that defect planes may shift off their ideal lattice positions, an effect for which we have not accounted in the DFT results.) Defect energies were computed from

\[
\gamma = \frac{E_{\text{defect}} - E_{\text{perfect}}}{m \|\mathbf{T}_1 \times \mathbf{T}_2\|} \tag{4}
\]

for \(m\) defect planes per unit cell. Each unit cell contained two defect planes, so that orthogonal translation vectors \(\mathbf{T}_{1,2,3}\) could be used as coordinate axes along the defect plane. In defective cells, two layers of atoms on each side of the defect plane were relaxed along \(\mathbf{T}_3\), with the cell shape and volume fixed to remove systematic errors. Specifically, the translation vectors were

\[
\begin{bmatrix}
\mathbf{T}_1 \\
\mathbf{T}_2 \\
\mathbf{T}_3
\end{bmatrix} = \begin{bmatrix}
1 & 1 & 0 \\
0 & 0 & 1 \\
8 & 8 & 0 \\
1 & 1 & 0 \\
2 & 2 & 4 \\
\end{bmatrix} \tag{5}
\]

Following Mehl et al.,\(^{29}\) we obtained the necessary elastic constants \(c_{ij}\) by solving for \(c_{44}, c' = (c_{11} - c_{12})/2,\) and bulk modulus \(B = (c_{11} + 2c_{12})/3\) through appropriate lattice distortion, where the Zener ratio \(A = c_{44}/c'\) and \(C = c_{44} .\) The total energy for each strain distortion in B2 is proportional to \(\varepsilon^2,\) with \(O(\varepsilon^3)\) error, giving more accurate coefficients. The Poisson ratio in Table I is computed from

\[
\nu = \frac{3B - 2G}{6B + 2G}. \tag{6}
\]

We provide in Table I the DFT and known observed values of all required quantities that are necessary in the maps that indicate enhanced ductility using elastic properties and relative defect energies.

IV. NECESSARY AND SUFFICIENT CONDITIONS FOR B2 DUCTILITY

We now derive the two conditions for ductility, applying them in Sec. V. Multiple slip can occur via formation of \{111\} APBs on the \{110\} and \{112\} planes. (For simplicity, the \(\frac{1}{2}\{111\}\{110\} and \frac{1}{2}\{111\}\{112\} APBs and \frac{1}{2}\{001\}\{110\} SFs are denoted as APB\{110\}, APB\{112\}, and SF\{110\}.) It is necessary, then, that the \{111\} APBs have to be more energetically favorable than the \{001\} SFs. To predict \{111\} versus \{001\} slip, Rachinger and Cottrell\(^{44}\) gave a simple criterion in terms of width of APB: \(w_{\text{APB}}/a > 1,\) then \{111\} slip is favorable; else if \(w_{\text{APB}}/a \approx 1,\) then \{001\} is favorable. We have derived a more quantitative necessary condition\(^{45}\) (see Appendix A) in light of Paidar, Pope, and Yamaguchi’s work in L1\(_2\) systems.\(^{14}\)

Saada and Veysseyre\(^{39}\) investigated the sufficient condition for cross-slip of a \{111\} screw superdislocation on \{110\} and \{112\} planes that leads to multiple-slip systems. The possible dissociation mechanisms for a \{111\} screw superdislocation are

\[
a(111) \rightarrow a(110) + a(001) \\
\rightarrow a(100) + a(010) + a(001), \tag{7a}
\]

\[
a(001) \rightarrow \frac{a}{2}(001) + SF + \frac{a}{2}(001), \tag{7b}
\]

\[
a(111) \rightarrow \frac{a}{2}(111) + \text{APB} + \frac{a}{2}(111). \tag{7c}
\]

In Eq. (7a), the \{111\} screw dislocation can further dissociate into perfect dislocations along the cube edges (Fig. 1); hence, there are no APBs or SFs. Equation (7b) involves formation of SFs.

A. Necessary condition

As described above, there are two criteria that must be met simultaneously that provide the necessary condition for ductility: \{001\} should be the dominant slip direction, yet \{111\} slip should also be possible with formation of \{111\} APBs; see Fig. 1. An overview of the derivation is provided in Appendix A.

On purely energetic grounds, for B2 materials to possess multiple slip during plastic flow, \{001\}\{110\} slip must be more favorable than \{111\}\{110\} slip via APB\{110\} formation, which occurs\(^{45}\) (see Appendix A) if

\[
w_{\text{APB}} \leq kea \sim 5.9a \quad \text{or} \quad \ln C \geq -3.9. \tag{8a}
\]

Equation (8) justifies the criterion imposed by Rachinger and Cottrell\(^{44}\) and gives a fixed measure across B2 systems. The second form is useful for presenting the maps.

Now, to have enhanced ductility, both \{001\} as the dominant slip direction, and \{111\} slip also possible by formation of \{111\} APBs, the APBs must be more energetically favorable than SFs. The key necessary condition\(^{45}\) (see Appendix A), using Eqs. (2) and (3), is

\[
\delta > 0.119C^{-1/4} \quad \text{or} \quad \ln \delta > -2.132 - \frac{1}{4} \ln C, \tag{9a}
\]

where the second form is easier for plotting the maps. Together Eqs. (8) and (9) constitute the map for B2 systems that will have both dominant \{001\} slip and \{111\} slip due to formation of APBs.

For our generic map and necessary conditions, as a standard simplification, we used a Poisson ratio of 1/3 (not values in Table I), which yields integer coefficients related to \(v.\) We also used an effective dislocation interaction range of twice the core width \(r = 2r_0 = 2ka;\) see Appendix A. While \(v = 1/3\) and the estimated \(k\) simplifies the algebra for the maps, the reader should appreciate that the exact borders for each material can be shifted by the actual values—the price for a generic map; hence, borderline cases should be assumed possibly relevant. Also, differences in various DFT calculations could alter locations in the maps, as we show explicitly.

B. Sufficient condition

As noted earlier, a ductile B2 material can have multiple slip only if APBs have bistable existence on both \{110\} and
TABLE I. Calculated and observed B2 lattice constants ($a$ in Å), bulk modulus ($B$ in GPa), and elastic constants ($c_{ij}$ in GPa). $A$, $\nu$, and $M$ are defined in the main text. In the first (second) row of each system, DFT calculations were performed at $a_{\text{DFT}}$ ($a_{\text{expt}}$). References for $a_{\text{expt}}$ are given in the second row. In the third row, $B$, $c'$, $A$, $\nu$, and $M$ were derived from the experimental elastic constants. Dashes indicate that no data are available.

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<th>$\nu$</th>
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\[ \lambda \equiv \frac{\gamma_{\text{APB}}^{112}}{\gamma_{\text{APB}}^{110}} \]  

and a ratio of \( S_{ij} \) elements

\[ M = \sqrt{\frac{S_{11}S_{44}}{S_{11}S_{44} - S_{15}^2}} \]  

See Ref. 47 for the full derivation of \( M \) and the definition of \( S_{ij} \), which are obtained by a rotation of the \( c_{ij} \) from cubic axes to the \( \langle 111 \rangle \) axis, as we also present in Appendix B. To satisfy the sufficient condition, expressed in terms of a dimensionless map (\( \lambda \) versus \( M \)), the \( \lambda \) must be strictly bounded as

\[ \frac{\sqrt{3}}{2} \leq \lambda \leq \frac{2}{\sqrt{3}} \]  

Within this bound, Sun found that both slip directions are active, but \( (1\bar{1}0) \) is dominant for \( M_1/3 < \lambda < 2/\sqrt{3} \) while \( (1\bar{1}2) \) is dominant for \( \sqrt{3}/2 < \lambda < M_1/3 \).

C. Prediction from combined maps

As the major results, we now have the necessary and sufficient conditions for enhanced B2 ductility. First, our more quantitative “Rachinger-Cottrell” criterion, Eq. (8), is used to predict dominant \( \langle 00\overline{1} \rangle \) slip. Then, on the same map, Eq. (9) compares the relative stability of APB\( \langle 11\overline{0} \rangle \) and SF\( \langle 11\overline{0} \rangle \) so that, if APBs are favorable, the systems possessing both \( \langle 00\overline{1} \rangle \) and \( \langle 11\overline{1} \rangle \) slip directions satisfy the necessary condition for ductility. Second, multiple slip in \( \{1\bar{1}0\} \) and \( \{1\bar{1}2\} \) via APB formation is governed by the sufficient condition [Eq. (12)] in a second map. Practically, if the necessary condition is fulfilled (the first map), then the sufficient condition is checked (the second map) for whether the material possesses bistability of APBs, and, hence, multiple slip can occur for enhanced ductility. We now use these to predict ductility for several B2 systems.

V. RESULTS

A. Necessary condition

A necessary condition map is constructed in Fig. 3. The dimensionless ratios \( C \) and \( \delta \) are defined in Eqs. (2) and (3), respectively. From Eq. (10) in Appendix A, it is shown that

\[ \ln \delta \text{ versus } \ln C \]
Eq. (8) can be expressed in terms of $C$. This condition translates to the vertical line drawn in Fig. 3, where (001) slip ([111] slip) is more favorable for systems lying to the right (left). Equation (9) translates to the slanted line in Fig. 3. Therefore, the necessary condition is satisfied in the upper-right region defined by these two lines, in which (001) is the dominant slip direction and formation of APBs, rather than SFs, is preferred. We note that the data in Fig. 3 lie along a line of slope slightly less than $-1$.

Systems favoring (001) slip include all the ionic compounds, all the Y-based compounds except for YMg, all the Sc-based compounds except for ScRu, and NiAl. Notably, ScPt is ductile but just barely predicted to be brittle from our analytic necessary conditions, a result that does depend on the accuracy of the DFT-derived inputs, or the underlying simplifications. For example, ScPt in Fig. 3 does satisfy the necessary conditions if $k \approx 4$ (rather than the $k = 2.17$ we assumed for all alloys, but it is in the acceptable range; see Appendix A). For $k \approx 4$, the APB versus SF slanted line shifts slightly down but parallel to the $k = 2.17$ line and ScPt falls in the upper-right region.

Ionic compounds are expected to exhibit (001) slip because ions encounter lower charge repulsion as they slip along cubic edges rather than cube diagonals. CuZn and FeAl fall on the left-hand side of the vertical line, showing that (111) slip is favorable, agreeing with their observed exclusive (111) slip. Interestingly, both (111) slip and (001) slip have been observed in AgMg, with a transition from (111) to (001) slip at low temperatures. For AuZn ($\lambda \approx 7.5$), the predicted (111) slip does not agree with the reported (001) slip, and further investigation is required. From Table I the largest errors in our calculated elastic constants are found in AuCd; we have omitted it from our ductility maps. The discrepancies observed in the two Au compounds may be caused by the usage of nonrelativistic pseudopotentials. It has been shown that relativistic effects play an important role in the bonding of Au clusters and may also pertain to the study of bulk compounds. For all the other systems, our simple model predicts (001) versus (111) slip accurately.

Figure 3 also compares the relative stability of SF[110] and APB[110]. For the ionic compounds, SFs are more stable than APBs. Charge repulsion in the APB is much higher than that in the SF. (See Table II for the calculated planar defect energies.) On the other hand, APBs are relatively stable in both the Y-based compounds and the classic B2 alloys.

Systems in the upper-right region, as defined by the vertical and slanted lines, of Fig. 3 satisfy the necessary condition for ductility. In this region, (001) slip is favorable but (111) APBs are stable, which means that $\lambda (111)$ partial dislocations can coexist with the (111)-dissociated perfect (001) dislocations. Indeed, it has been reported that (111) dislocations are metastable in NiAl and that they have been observed in the Y-based compounds.

The first central finding is that the B2 stability map in Fig. 3 identifies candidates for multiple slip, and only a subset of Y- and Sc-based systems and some others qualify, namely, YAg, YCu, YIn, YRh, YZn, ScAg, ScAu, ScCu, Cspd, (ScPt), ScRh, NiAl, CsI, and (CsCl), where the parentheses reflect a borderline case that should be checked.

**B. Sufficient condition**

The necessary condition alone cannot predict ductility. The sufficient condition (Fig. 4)—whether the APBs are bistable on [110] and [112] planes—must be verified. Dimensionless ratios $\lambda$ and $M$ are defined in Eqs. (10) and (11), respectively. The condition for bistability of APBs is satisfied in regions II and III, according to Eq. (12). In region II, the [110] APB has lower energy, and vice versa in region III (see Fig. 4).

![Figure 4](image-url)

**Fig.** 4. Left: Sufficient condition ($\lambda$ versus $M$) map for multiple slip systems [Eq. (12)] that occurs if $\sqrt{3}/2 < \lambda < 2/\sqrt{3}$. Materials not satisfying the necessary condition are marked by open diamonds. ScPt being the borderline case in Fig. 3, is marked by a half-filled diamond. DFT values of YCu and YAg reflecting energies from Ref. 10 are indicated by open circles. Right: Schematics showing the relative energy of the slip systems (after Ref. 48). Below $\lambda = \sqrt{3}/2 \approx 0.866$, only [112] slip is favored.
In regions I ($\lambda > 2/\sqrt{3}$) and IV ($\lambda < \sqrt{3}/2$, not shown), respectively, \{112\} and \{110\} APBs are unstable. ScRu is not shown as its $\lambda$ value falls out of range (Table II). ScCu satisfies the necessary condition and just barely does not satisfy the sufficient conditions; this borderline case is sensitive to DFT approximations. For example, a 1.4% increase in the $\gamma_{1\bar{1}0}^{\text{APB}}$, i.e., from 713 to 723 mJ/m$^2$, in Table II would put ScCu below the bistability line; hence, we include ScCu as ductile. The compounds that satisfy both the necessary and sufficient conditions are YAg, YRh, ScAu, ScAg, (ScPt), ScPd, (ScCu), and ScRh. For these B2 materials we predict enhanced ductility; all other compounds are predicted to be brittle.

Out of all the B2 systems, only YAg and YCu have been examined in other DFT calculations. There are two notable things: (1) elastic constants in Table I from our and Morris et al.'s results are the same and agree with experiment, but (2) the defect energies are significantly different in Table II. We have been unable to reproduce their defect energies for YCu, and for YAg the values are similar but swapped, changing the relative energies $\lambda$ in Fig. 4. If Morris et al.'s $\lambda$ values for YCu and YAg are plotted in Fig. 4, their locations both shift downward, with YCu (YAg) now in region II (III), and both (not just YAg) satisfy bistability explaining enhanced ductility.

The second central finding is that the sufficient condition shown in Fig. 4 identifies B2 materials that can exhibit multiple slip. Systems that do not satisfy the necessary condition are included for comparison. Only YAg, [YCu], YRh, ScAu, ScAg, (ScPt), ScPd, (ScCu), and ScRh possess \{110\} and \{112\} bistability, while other candidates lie away from the bistability region. Bracketed YCu reflects the unresolved DFT values. The bistability of APBs explains the observation of many $\langle 111 \rangle$ dislocations in the ductile Y-based and Sc-based compounds, even though $\langle 001 \rangle$ is the dominant slip direction.

VI. DISCUSSION

The systems that satisfy the necessary conditions (Fig. 3 showing dominant (001) slip existing with (111) slip and stable APBs, not SFs) and the sufficient condition (Fig. 4, regions II and III, showing APBs having bistable slip) are predicted to
have significant enhanced ductility unexpected in B2 systems. Borderline cases (if using DFT inputs) should be carefully addressed. It happens that none of the elastically anisotropic B2 materials satisfy both the necessary and sufficient conditions, explaining the observation of brittleness in all the classic B2 alloys, which are anisotropic. The ductile materials are all nearly isotropic. Hence, elastic isotropy ($A \sim 1$) should serve as an indicator for enhanced ductility. It is, however, not a quantitative indicator because $YCu$ is more isotropic than $YAg$, but $YCu$ is less ductile.

ScRu is predicted to be brittle, which agrees with experiment. ScAg, ScAu, and ScPd are correctly predicted to be ductile. ScPt is ductile but is a borderline case barely not satisfying the necessary condition. And, if we take ScPt to satisfy the necessary condition, then it is ductile because the sufficient condition is also satisfied. (If ScPt is taken to satisfy necessary condition, then so too should CsCl, but it does not satisfy the sufficient condition.) The Rh compounds YRh and ScRh are brittle but predicted to be ductile. Further investigation in this chemical space is required to understand the source of the discrepancy. As noted, the neglect of a shift of the defect planes from the ideal position, the sensitivity to the specific DFT exchange-correlation functional, or the neglect of other defect formations may change these cases.

Not all Y-based compounds are predicted to be ductile: B2 YIn does not satisfy the sufficient condition (similar to AuZn, $A \sim 7.5$, which means that it is not very isotropically elastic); YMg does not satisfy the necessary condition, so it is brittle, as found experimentally. YIn has been observed to form a B2 phase. However, YIn has been reported to crystallize also into a tetragonal phase, which is ductile. Our DFT calculations (unpublished) show that YIn has a shallow energy trough versus $c/a$ making it susceptible to $c/a$ distortion depending on sample treatment. Thus, while the B2 YIn is brittle from our theory for B2 ductility (using our DFT results), if $c/a$ distortion occurs, a more general ductility criterion for the dislocation-defect reactions should be derived accounting for $c/a$ dependence.

Finally, regarding correlation of measured ductility with $d$-electron density of states (DOS), we note that our theory addresses the ductility criterion based on defect energies and elastic constants that inherently reflect the bonding represented within DFT, as did the theory of Liu et al. on yield-strength anomalies in L1$_2$ compounds. A similar approach for quantitative prediction of twinning in elements and solid-solution alloys (based on the interacting dislocation and planar-defect arrays in a twin nucleus) also reflect bonding, which can be correlated directly to the electronic structure. As noted above, a significant (but not absolute) correlation of calculated $d$-electron DOS at the Fermi energy was cited for B2 alloys that were measured to have little to no ductility. Importantly, from our maps for the necessary and sufficient conditions (using our DFT results), we can predict ductility and, if desired, attempt to correlate behavior with the DFT-derived DOS.

In Fig. 5, we show the DOS for B2 ScRu (brittle), ScRh (predicted ductile, observed brittle), and ScPd and ScAg (both ductile) in order of increasing electron-per-atom ratio, or $e/a$. ScRu has the largest $d$-state DOS at the Fermi level and correlates with the predicted/observed lack of ductility. ScRh, with its extra electron over ScRu, is in low-$d$-state DOS between bonding and antibonding $d$ states, which suggests a crossover in bonding behavior—not incompatible with the present results taken in toto. Both ScPd and ScAg are ductile, with the Fermi energy beginning to climb into higher $d$-band DOS and the bonding peak of the $d$-band DOS falling farther below the Fermi energy. These results appear to agree with the results of Gschneidner et al., but their DOS contains no detail to make any direct comparison. They argue only that a broad $d$-band DOS at the Fermi energy explains the lack of ductility, whereas, for ScPd and ScAg, this $d$-band feature is farther below the Fermi energy and accounts for ductility; how it does so is not explained. Of course, that the Fermi energy is entering the DOS with antibonding character should make ductility, i.e., defect formation, more energetically favorable, as inherently represented in the present theory. We can correlate our predicted brittleness, brittle-to-ductile crossover, and ductility with the change in DOS features. Thus, we agree that the magnitude of the $d$-band DOS at the Fermi energy can be correlated with ductility if already known, but such a correlation by itself is not predictive theory. Indeed, the change in DOS under shear is more relevant, as is known for aluminum; for example, $s$ bonds under shear become very directional, giving rise to a large stacking fault energy, as observed. Hence, investigating the behavior of the charge density under shear may be more fruitful than DOS.

Finally, for completeness, we note that the underlying theory for higher ductility is generally more complicated than the simple dissociations present here as a starting analysis. That is, there are key factors determining slip systems, e.g., elastic anisotropy, the “correct” vectors of possible faults in (101) planes (not always corresponding to the usually presumed APBs), and the energies of these faults. So, it is possible that the splittings could be different from the usual APBs considered here. As a starting point, if all B2 systems are treated equally, we assume that there are well-defined APBs on {110} and {112} planes with the displacement vector $\frac{1}{2}(111)$ and also a stacking fault on {110} planes with the vector $\frac{1}{4}(001)$. However, the existence of such metastable faults is by no means guaranteed—indeed they are system specific. The metastability of such faults is the crucial condition for any further considerations employing standard (anisotropic) dislocation theory. The symmetry does not provide a guarantee of the stability of these faults. On {110} planes there may be metastable $\frac{1}{2}(111)$ faults in some materials, e.g., CuZn or FeTi. However, the vectors corresponding to metastable faults may differ from $\frac{1}{2}(111)$; for example, simulations using empirical potentials found in NiAl that the APB with $\frac{1}{2}(111)$ is not actually stable but other faults on {110} planes existed. The point is that vectors of the faults on {110} planes vary from material to material and are by no means the same in all B2 compounds.

Nonetheless, the present stability analysis provides a very rapid analysis to identify and reduce the number of candidate anomalously ductile B2 systems, and, from which, one can consider other, more atypical, instabilities. For future work, we can investigate the metastability of the planar defects addressed in the present simplest theory, since they may be unstable with respect to other defects on the activated slip planes. If so, the dissociation mechanisms considered here would then be
STABILITY MAPS TO PREDICT ANOMALOUS DUCTILITY

VII. CONCLUSIONS

Through solely energy-based criteria for ductility (dislocation and defect formation), we have addressed (001) versus ⟨111⟩ slip, the relative stability of APBs and SFs, and the bistability of APB{110} and {112}, which are the dominant slip modes and defects in B2 systems that can lead to enhanced ductility. Through these criteria, we have provided a set of stability maps requiring only ratios of defect energies and/or elastic constants, obtained here from DFT calculations. For design, these maps determine a priori whether a B2 material is brittle or ductile and indicate typical versus enhanced ductility. These maps explain and predict the enhanced ductility observed (or lack thereof) in RM intermetallic compounds. One may consider temperature effects, point defects, or disorder to modify the maps for system-specific predictions, as well as more system-specific superdislocation reactions that we did not consider.

We have examined 23 B2 materials, some of which show dramatically enhanced ductility, comparable to fcc aluminum. For B2 materials, ⟨001⟩ slip is more favorable than ⟨111⟩ if the width of APB{110} is less than 6a. To summarize our results from the B2 stability maps:

1. For ionic compounds, only ⟨001⟩ slip is possible, as the necessary condition for ductility is not satisfied. If the borderline CsI were assumed to satisfy the necessary condition, the lack of APB bistability would account for its brittleness.

2. For classic B2 alloys, all but NiAl fail the necessary condition. Again, APBs of NiAl do not possess bistability (multiple slip) so there is no increased ductility.

3. For Y- and Sc-based compounds, YA, YRh, ScAg, ScAu, (ScPt), ScPd, (ScCu), and ScRh satisfy both conditions for multiple-slip systems. Thus, we predict them to exhibit high ductility (observed for YA). YIn and YMg do not satisfy either condition, so they are predicted to be brittle (observed in YMg), while B2 YIn has competing tetragonal distortions that will affect prediction.

4. We predicted some systems, such as ScRh, that are ductile but brittle; these appear at a crossover, e.g., between ScRu and...
strain field is canceled by the strain field of other dislocations. The pure screw-screw and edge-edge interaction energies are

\[ E_{ss} = \frac{G b_s^2}{2\pi} \ln \frac{r}{w}, \]  

\[ E_{ee} = \frac{G b_e^2}{2\pi(1-v)} \ln \frac{r}{w}, \]  

where \( w \) is the separation distance between APBs or SFs.

In Eq. (7a) of the main text, the (111) screw dislocation dissociates into perfect dislocations along the cube edges; hence, there are no APBs or SFs. The dissociation does not result in any change in the total energy. Thus, with \( b_{a,s} = a(111) \) and \( b_{a,e}^2 = 3a^2 \), the total energy of the screw dislocation is

\[ E_a = \frac{G b_{a,s}^2}{4\pi} \ln \frac{r}{r_0} = \frac{3Ga^2}{4\pi} \ln \frac{r}{r_0}. \]  

In Eq. (7c) of the main text, the (111) screw dislocation can dissociate into two \( \frac{1}{2} \langle 111 \rangle \) partials bounding an APB. The partials are purely screw, with Burgers vector \( b_{c,s} = \frac{a}{2}(111) \) and \( b_{c,e}^2 = 3a^2/4 \). Given the separation width \( w_{APB} \) of the partials, with planar defect energy \( \gamma_{APB} \), the total energy is

\[ E_c = 2E_{c,s} + E_{c,ee} + \gamma_{APB} w_{APB}. \]  

We minimize the energy with respect to \( w_{APB} \), from which we find that

\[ w_{APB} = \frac{G b_{c,s}^2}{4\pi \gamma_{APB}} = \frac{3Ga^2}{8\pi \gamma_{APB}}. \]  

Then, purely on energy grounds, in order for \( \langle 001 \rangle \langle 110 \rangle \) slip to be more favorable than APB\{1\bar{1}0\} formation, \( E_a \) in Eq. (A5) must be less than \( E_c \) in Eq. (A6):

\[ \frac{3Ga^2}{4\pi} \ln \frac{r}{r_0} < \frac{3Ga^2}{8\pi} \left( \ln \frac{r}{r_0} + \ln \frac{r}{w_{APB}} + 1 \right) \]  

or

\[ \ln \frac{w_{APB}}{r_0} < 1. \]  

The dislocation core is \( r_0 = ka \) for some constant \( k \). Then, by Eq. (A8), the condition for \( \langle 001 \rangle \) slip is

\[ \frac{w_{110}^{110}}{a} < k e, \]  

or, in terms of the planar defect energy, as

\[ \frac{\gamma_{APB}^{110}}{Ga} > \frac{3}{8\pi ke}, \]  

or

\[ \ln C > \ln \left( \frac{3}{8\pi ke} \right) \sim -3.126 - \ln k. \]  

The core of the dislocation can be simulated using semiempirical and first-principles calculations, from which the radius of the core, and hence \( k \), can be obtained for each B2 material. In general, \( r_0 \) has a range of \( b \) to \( 5b \), so \( k \) is between \( \sqrt{5}/2 \) and \( 5\sqrt{3}/2 \) in our case. Eshelby estimated analytically \( r_0 \) to be about 1.5\( b \) for screw dislocations, which, according to Read, is an underestimate. A simulation study by Xu and Moriarty shows that \( 2b \), where \( b = \frac{a}{2}(111) \), is a good approximation for \( r_0 \) in bcc Mo. We expect the core radius to be somewhat larger in B2 systems than in bcc metals, since a represents a partial dislocation in B2 instead of a perfect
the partial dislocation can be found by projecting $S_{ij}$ for comparison of many systems.

The derivation of the necessary [Eq. (9)] condition, $\delta > 0.119C^{-1/4}$, is more involved. It results from an energy-based comparison between APB and SF planar defect energies.\textsuperscript{45} Equation (7b) shows that the $a$(001) dislocation can further dissociate into $\frac{1}{2}$(001) partial dislocations, creating a super-intrinsic stacking fault. The screw and edge components of the partial dislocation can be found by projecting $\frac{1}{2}$(001) onto $a$.(111):

$$\frac{a}{2}(001) = \frac{a}{6}(111) + \frac{a}{6}(\bar{1}1\bar{2}). \quad (A11)$$

Thus, with $b_{h,k}^2 = a^2/12$ and $b_{h,k}^2 = a^2/6$, and using the self-energies from Eqs. (A1) and (A2) and the interaction energies from Eqs. (A3) and (A4), the total energy associated with SF formation is

$$E_b = \frac{Ga^2}{24\pi} \left( \ln \frac{r}{r_0} + \ln \frac{r}{w_{\text{SF}}} \right)$$

$$+ \frac{Ga^2}{12\pi(1-\nu)} \left( \ln \frac{r}{r_0} + \ln \frac{r}{w_{\text{SF}}} \right) + \gamma_{\text{SF}}w_{\text{SF}}. \quad (A12)$$

Minimizing energy with respect to $w_{\text{SF}}$, the separation width is found to be

$$w_{\text{SF}} = \frac{3 - \nu}{1-\nu} \frac{Ga^2}{24\pi\gamma_{\text{SF}}}. \quad (A13)$$

Then Eq. (A12) becomes, with $\nu = 1/3$,

$$E_b = \frac{3 - \nu}{1-\nu} \frac{Ga^2}{24\pi} \left( \ln \frac{r}{r_0} + \ln \frac{r}{w_{\text{SF}}} + 1 \right). \quad (A14)$$

Finally, we compare SF formation [Eq. (7b)] with APB formation [Eq. (7c)]. Note, we must multiply $E_b$ by 3 for a fair comparison, since each (111) dislocation dissociates into three families of (001) dislocations, where each of them can create SFs independently. So, for APBs to be more energetically favorable than SFs, we need $E_c$ in Eq. (A6) to be less than $3E_b$ in Eq. (A14); i.e.,

$$3 \ln \frac{r}{w_{\text{APB}}} - \frac{2\nu}{1-\nu} \left( 1 + \ln \frac{r}{r_0} \right) < \frac{3 - \nu}{1-\nu} \ln \frac{r}{w_{\text{SF}}}. \quad (A15)$$

With $r_0 = ka$, and assuming consistently that $\nu = 1/3$ and $r = 2r_0 \approx 4.33a$, we get a criterion for APB formation to be more favorable than SF formation, i.e., Eq. (9).

**APPENDIX B: ELASTIC CONSTANTS FOR BISTABILITY MAP**

Here we provide an overview of how compliance elements $S_{ij}$ are related to standard elastic constants $c_{ij}$. The derivations can be found by combining information in Refs. \textsuperscript{46} and \textsuperscript{47}.

Bistability is determined by the anisotropic elastic response of the B2 lattice. $M$ is a function of $c_{ij}$:\textsuperscript{46,47} Let $H = 2c_{44} + c_{12} - c_{11}(c_{11} - c_{12})(A - 1)$, where $A$ is the Zener ratio, Eq. (1). Rotating the cubic elastic constants to the [111] axis yields

$$c'_{ij} = \begin{bmatrix} c'_{11} & c'_{12} & c'_{13} & 0 & c'_{15} & 0 \\ c'_{12} & c'_{11} & c'_{13} & 0 & -c'_{15} & 0 \\ c'_{13} & c'_{13} & c'_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c'_{44} & 0 & -c'_{15} \\ c'_{15} & -c'_{15} & 0 & 0 & c'_{44} & 0 \\ 0 & 0 & 0 & -c'_{15} & 0 & c'_{66} \end{bmatrix}, \quad (B1)$$

where

$$c'_{11} = c_{11} + \frac{1}{2}H, \quad c'_{12} = c_{12} - \frac{1}{6}H, \quad c'_{13} = c_{12} - \frac{1}{3}H, \quad c'_{33} = c_{11} + \frac{2}{3}H, \quad c'_{44} = c_{44} - \frac{1}{6}H, \quad c'_{66} = c_{44} - \frac{1}{6}H, \quad c'_{15} = -\frac{\sqrt{2}}{6}H.$$\textsuperscript{46,47}

Note, for an isotropic material, $A = 1$, $H = 0$, and $c'_{ij} = c_{ij}$. The third row and column are deleted to obtain the inverse,\textsuperscript{46} yielding

$$S_{ij} = \begin{bmatrix} S_{11} & S_{12} & 0 & S_{15} & 0 \\ S_{12} & S_{11} & 0 & -S_{15} & 0 \\ 0 & 0 & S_{44} & 0 & -2S_{15} \\ S_{15} & -S_{15} & 0 & S_{44} & 0 \\ 0 & 0 & -2S_{15} & 0 & S_{66} \end{bmatrix}, \quad (B2)$$

where

$$S_{11} = c'_{11}c'_{44} - c'_{15}^2 / 2(c'_{11} + c'_{12})(c'_{44}c'_{66} - c'_{15}^2),$$

$$S_{12} = c'_{12}c'_{44} + c'_{15}^2 / 2(c'_{11} + c'_{12})(c'_{44}c'_{66} - c'_{15}^2),$$

$$S_{44} = c'_{44}c'_{66} - c'_{15}^2, \quad S_{66} = c'_{44}c'_{66} - c'_{15}^2,$$

$$S_{15} = -c'_{15}^2 / 2(c'_{44}c'_{66} - c'_{15}^2).$$

Finally, the parameter $M$ is defined as

$$M = \sqrt{\frac{S_{11}S_{44}}{S_{11}S_{44} - S_{15}^2}}. \quad (B3)$$

As discussed by Sun,\textsuperscript{48} $M \geq 1$, where the equality holds only for isotropic materials, where $A = 0$ and, hence, $H = 0$. 

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J. R. Morris and Y. Y. Ye (private communication).


