Ideal strength and intrinsic ductility in metals and alloys higher-order elastic constants

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Under tensile loading the ideal strength of a solid is governed by mechanical instabilities corresponding to failure in tension or shear, indicative of intrinsic brittle or ductile behavior, respectively. First principles-calculations for hexagonal-close-packed (hcp), face-cemtered-cubic (fcc) and body-centered-cubic (bcc) metals and alloys are used in this work to divide up the periodic table in two classes, corresponding to intrinsically brittle or ductile materials. An analytical model is developed that accurately predicts ideal deformation behavior and the failure modes based on knowledge of just the standard second-order and third-order elastic constants. For the transition metals, filling of the d-bands is shown to correlate with the type of instability realized, thus providing unique insights into the effect of alloying on the intrinsic mechanical behavior of hcp metals.

I. INTRODUCTION

Intro goes here

II. METHODOLOGY

A. Deformed elastic constants

Eqs. 1 denote the deformed elastic constants for cubic crystals under c-loading. Eqs. 2 denote the deformed elastic constants for hexagonal crystals under c-loading. In Eqs. 1 and 2, ξ is the strain along c and η is the strain in the a-b plane, perpendicular to the c-direction. The terms C_{ij} represent the standard second-order elastic constants (SOEC's) and the terms C_{ijk} represent the third-order elastic constants (TOEC's).

$$C'_{11} = C_{11} + \eta\left(3C_{11} + C_{12} + C_{111} + C_{112}\right) + \xi\left(-C_{11} + C_{12} + C_{112}\right), \tag{1a}$$
$$C'_{12} = C_{12} + \eta\left(-C_{11} + C_{12} + 2C_{112}\right) + \xi\left(-2C_{12} + C_{123}\right), \tag{1b}$$
$$C'_{13} = C_{12} + \eta\left(-C_{11} - C_{12} + C_{112} + C_{123}\right) + \xi C_{112}, \tag{1c}$$
$$C'_{33} = C_{11} + \eta\left(-3C_{11} + 3C_{12} + 2C_{112}\right) + \xi\left(5C_{11} - C_{12} + C_{111}\right), \tag{1d}$$
$$C'_{44} = C_{44} + \eta\left(\frac{1}{2}C_{11} + \frac{3}{2}C_{12} + C_{144} + C_{166}\right) + \xi\left(\frac{1}{2}C_{11} + \frac{1}{2}C_{12} + C_{44} + C_{166}\right), \tag{1e}$$
$$C'_{66} = C_{44} + \eta\left(C_{11} + C_{12} + 2C_{44} + 2C_{166}\right) + \xi\left(C_{12} - C_{44} + C_{144}\right) \tag{1f}$$

$$C'_{11} = C_{11} + \eta\left(3C_{11} + C_{12} + 2C_{222} - 3C_{661} - C_{662}\right) + \xi\left(-C_{11} + C_{23} + C_{223}\right), \tag{2a}$$
$$C'_{12} = C_{12} + \eta\left(-C_{11} + C_{12} + 2C_{222} - 5C_{661} - 3C_{662}\right) + \xi\left(-C_{12} + C_{223} - C_{23} - 2C_{663}\right), \tag{2b}$$
$$C'_{23} = C_{23} + \eta\left(-C_{11} - C_{12} + 2C_{223} - 2C_{663}\right) + \xi\left(C_{332}\right), \tag{2c}$$
$$C'_{33} = C_{33} + \eta\left(2C_{23} - 2C_{33} + 2C_{332}\right) + \xi\left(4C_{33} + C_{333}\right), \tag{2d}$$
$$C'_{44} = C_{44} + \eta\left(\frac{1}{2}C_{11} + \frac{1}{2}C_{12} + C_{23} + C_{551} + C_{552}\right) + \xi\left(\frac{1}{2}C_{23} + \frac{1}{2}C_{33} + C_{44} + C_{553}\right), \tag{2e}$$
$$C'_{66} = \frac{1}{2}\left(C'_{11} - C'_{12}\right) \tag{2f}$$

B. Wallace formalism and elastic instabilities

The elastic stability of a solid under zero stress is governed by the eigenvalues of its elastic-constant tensor; specifically, all 6 eigenvalues of this tensor must be larger than zero for the solid to be elastically stable. For a solid under an applied stress, elastic stability is governed instead by the Wallace tensor, defined as follows:

$$B_{ijkl} = C'_{ijkl} + \frac{1}{2}\left(\sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik} + \sigma_{ik}\delta_{jl} + \sigma_{jk}\delta_{il} - 2\sigma_{ij}\delta_{kl}\right) \quad (3)$$

where C'_{ijkl} represents the elastic constants in the deformed configuration[1–3], σ_{ij} denotes the applied stress acting on the solid, and δ_{ij} is the Kronecker-delta. The eigenvalues of the symmetrized Wallace tensor govern the elastic stability of a solid under stress[4]. In the present context, the symmetrized Wallace tensor, B_{sym} is defined as $B_{sym} = 1/2\ (B + B^T)$ (with B given in Eq. 3), where the use of Voigt notation is implied so that both B and B_{sym} reduce to 6×6 matrices. In the remainder of this paper, the Wallace-tensor B_{ijkl} refers to the symmetrized Wallace tensor.

Elastic instabilities are studied in this work by computing the Wallace tensor (Eq. 3) as a function of strain ξ. The deformed elastic constants C'_{ijkl} are calculated directly from Eqs. 1 and 2. The Cauchy stress σ_{ij} can be expressed in terms of the applied strain and the deformed elastic constants, as shown in the Supplemental Material. This formalism allows to analytically calculate the ideal deformation behavior of materials based on just a knowledge of the SOEC's and TOEC's.

C. Calculations of second-order and higher-order elastic constants

- Describe how SOEC's and TOEC's are calculated.
- Refer to SM for details.

D. DFT calculations

- Describe DFT calculations in detail.
- Describe Virtual Crystal calculations.

E. Alloys and SQS generation

- Describe SQS procedure generation here.
- Discuss rationale for looking at B2 Mo-Nb.

III. RESULTS AND DISCUSSION

A. Elastic instabilities and intrinsic ductility

B. Elastic instabilities and d-band filling

IV. SUMMARY AND CONCLUSIONS

[1] D. C. Wallace, Thermodynamics of crystals (Courier Corporation, 1998).
[2] J. R. Ray, Computer physics reports **8**, 109 (1988).
[3] J. Wang, S. Yip, S. Phillpot, and D. Wolf, Physical Review Letters **71**, 4182 (1993).
[4] J. Wang, J. Li, S. Yip, S. Phillpot, and D. Wolf, Physical Review B **52**, 12627 (1995).

TABLE I. Calculated SOEC's, TOEC's and ideal-failure characteristics for selected cubic metals and intermetallics. Failure modes are characterized as either shear (S) or tension (T).

	Mo	Nb	W	Ta	B2-MoNb
SOEC's (GPa)					
C_{11}	462	265	516	271	334
C_{12}	171	126	215	168	127
C_{44}	85	25	134	71	47
TOEC's (GPa)					
C_{111}	-4688	-1812	-5613	-2567	-3294
C_{112}	-974	-233	-967	-1116	-948
C_{123}	-37	-1221	-420	1024	317
C_{144}	-447	-540	-848	-298	-239
C_{155}	-756	11	-816	-625	-683
C_{456}	-176	207	-571	40	-144
Failure characteristics					
Failure mode	tension	shear	tension	shear	shear
Eigenvector (approx.)	$(0,0,1,0,0,0)$	$(0,0,0,0,0,1)$	$(0,0,1,0,0,0)$	$\left(\frac{1}{2}\sqrt{2},-\frac{1}{2}\sqrt{2},0,0,0,0\right)$	$(0,0,0,0,1,0)$

TABLE II. Calculated SOEC's, TOEC's and ideal-failure characteristics for 12 HCP metals. Failure modes are characterized as either shear (S) or tension (T). [Rerunning these calculations now]

	Sc	Y	Ti	Hf	Zr	Tc	Re	Ru	Os	Zn	Mg	Be
SOEC's (GPa)												
C_{11}	100	77	174	182	145	489	618	554	733	166	59	306
C_{12}	37	25	81	72	64	225	275	181	227	36	29	32
C_{13}	29	27	75	69	66	192	224	176	225	35	20	15
C_{44}	29	25	43	52	25	171	159	175	248	30	17	165
C_{33}	71	61	183	20	161	534	677	613	801	71	67	406
TOEC's (GPa)												
C_{133}	-117	-143	-273	-214	-146	-1014	-1557	-1220	-1408	-21	-1808	-318
C_{333}	-230	-303	-1078	-1463	-1173	-4004	-5715	-5980	-7955	-797	-4625	-4347
C_{111}	-734	-529	-1584	-1567	-1301	-4771	-6786	-5758	-7764	-2179	-5247	-2407
C_{112}	-83	-24	10	-120	103	-526	-1020	-656	-828	-57	-1531	-81
C_{113}	-50	-58	169	-22	169	6	107	-621	-604	31	432	59
C_{222}	-691	-475	-1173	-1354	-961	-4175	-6103	-5263	-7146	-2862	-5043	-1887
C_{123}	-219	-185	-661	-237	-494	-1768	-712	-275	-332	-498	-1886	-7
C_{144}	-15	8	170	-260	218	-1100	-451	-417	-562	-227	-964	-332
C_{155}	37	58	-34	-154	49	-126	-519	-566	-801	-351	8	-88
C_{344}	-135	-128	-246	-460	-162	-1061	-1281	-930	-1297	-234	-727	-726
Failure characteristics												
$\bar{\xi}$ (direct DFT)	0.22	0.20	0.19	0.14	0.19	0.18	0.19	0.15	0.15	0.12	0.22	0.17
$\bar{\xi}$ (analytical)	0.30	0.26	0.24	0.20	0.15	0.19	0.24	0.18	0.19	0.13	0.24	0.16
σ_{id} (GPa) (direct DFT)	13	9	15	12	11	44	54	48	62	5	6	24
σ_{id} (GPa) (analytical)	11	8	13	10	8	36	44	33	42	3	5	20
Failure mode	S	S	S	S	S	S	S	T	T	T	T	T