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Physics of the Lindemann melting rule

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Abstract We investigate the thermodynamics of melting for 74 distinct chemical elements including several actinides and rare earths. We find that the observed melting points are consistent with a linear relationship between the correlation entropy of the liquid and the Grüneisen constant of the solid, and that the Lindemann rule is well obeyed for the elements with simple structures and less well obeyed for the less symmetric more open structures. No special assumptions are required to explain the melting points of the rare earths or light actinides.

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1. Introduction

The melting point varies over a wide range across the periodic table. This is shown in figure 1, drawn in the highly informative format introduced by Sanderson [1]. It it desirable to have a reliable means of predicting the melting points of materials on the basis of known physical properties. A widely used melting criterion grew out of work published by Lindemann [2] in 1910 and modernized by Gilvarry [3]: a material melts at that temperature for which the amplitude of thermal vibration is a certain fraction f of the interatomic distance in the crystal. The quantity f is not specified precisely, but is in the range of 5-15%. An interesting history of the Lindemann melting rule has been given by Wallace [4,5].

The Lindemann rule has powerful intuitive appeal. At high enough temperatures, we can imagine that the crystal must "shake itself to pieces," in the picturesque language of F. C. Frank [6]. At low temperatures, the crystal is nearly static, and the thermal vibrations are irrelevant. The melting point is somewhere in between; a critical amplitude characterized by a fraction $\approx 10\%$ is not unreasonable.

The Lindemann rule has been used for estimation of the melting point with considerable success for many years, but is open to criticism on at least three fronts. First, the stated rule does not have a legitimate physical basis, as the vibrational amplitude is a property of the *solid* alone, and *liquid* state is not explicitly considered; a proper thermodynamic model would consider *both* states [7]. Second, the critical fraction f is only vaguely specified. Finally, the accuracy of the rule is poor, in the range of 20-25%. The Lindemann rule remains in use because there is nothing better.

The first criticism has been addressed by several workers, particularly Wallace. [4,5,8] Wallace works from the entropy balance at the melting transition:

$$S_{liquid} - S_{solid} = \Delta S \qquad (1)$$

ΔS is the measured entropy of melting which is found to be $1.1 k_B$ per atom on average; this is Richard's rule [9], (We will subsequently express the entropy in units of k_B, the Boltzmann constant.) For the liquid, Wallace writes

$$S_{liq,W} = \frac{3}{2} \ln \left[\frac{k_B Te}{\left(\frac{2\pi\hbar^2}{M\Omega^{\frac{2}{3}}} \right)} \right] + S_{corr} = \frac{3}{2} \ln \left[\frac{k_B TM\Omega^{\frac{2}{3}} e}{2\pi\hbar^2} \right] + S_{corr} = S_{S-T} + S_{corr} \tag{2}$$

The first term of Wallace's entropy is just the Sakur-Tetrode entropy for an ideal gas with the available volume replaced by the finite, fixed atomic volume . (Here we use the subscript W to distinguish Wallace's expressions from slightly different ones that we will use later.) In this expression, Ω is the atomic volume, M is that atomic mass, e is the base of natural logarithms, $\hbar$ is Planck's constant divided by 2π, and $S_{corr,W}$ is the extra (negative) entropy arising form the correlation of atomic motion in the liquid state. Wallace has carefully mined the available pair correlation data derived from x-ray and neutron scattering experiments on liquid metals and determined that the correlation entropy may be expressed as $S_{corr,W} = X + Y \ln(T/T_M)$, where X and Y are material-specific constants [5,8]. As an average, he finds $S_{corr,W} = -2.6 + 1.7 \ln(T/T_M)$

For the solid, he uses $S_{sol,W} = 3\ln(Te/\Theta_0)$, where Θ_0 is the characteristic entropy temperature, the zero-th moment of the phonon spectrum. In addition, one must consider a correction for vibrational anharmonicity. Wallace shows that this is not readily obtained from first-principles theory, but is fortunately negligible. In the end, he obtains a satisfactory account of the melting temperatures of the 30 elements he is able to treat by rigorous methods, which are unfortunately limited by the availability of data for the determination of Θ_0 and $S_{corr,W}$. Wallace also identifies a group of "anomalous" elements, for which a simple melting criterion based on equation (1) is not successful, and suggests that these

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elements undergo an additional electronic transition at the melting point. He includes in this group: Sn, Ga, Sb, Bi, Si and Ge.

In subsequent sections of this paper we use an empirical approach that is less rigorous than Wallace's. We will be able to consider more than 70 elements, including some of the actinides, and to point out and important property of the correlation entropy.

2. Entropy, melting point and atomic vibrations

The energy $k_B T_M$, where T_M is the melting point and k_B is the Boltzmann constant, is a useful dimensionless number when divided by the characteristic elastic energy, $B\Omega$, where B is the bulk modulus and Ω the atomic volume. Another useful parameter is the dimensionless thermal expansion defined by $\gamma = \beta B\Omega/C_V$, where β is the volume thermal expansion, B is the bulk modulus, Ω is the atomic volume, and C_V is the heat capacity per atom. This is the Grüneisen γ. All of these quantities may be temperature dependent, and then γ is. At high enough temperatures, C_V is just $3k_B$, and the temperature dependences of the other quantities cancel to a good approximation, and then γ may be taken as constant. [10,11]. As a dimensionless thermal expansion, γ is a useful parameter to characterize vibrational anharmonicity. For anisotropic materials, the γ we have defined here is not strictly valid [12], but we will use it anyway on a provisional basis. The necessary data for computing $k_B T_M/B\Omega$ and γ can be obtained in the literature. In our case, most of the data were found in the review of Gschneidner [13]. These data were supplemented in a few cases with more current results: α-Pu [14,15], δ-Pu [16], ϵ-Pu [17] γ-U [18,19] and γ-Ce [20]. In the case of δ-Pu, the anomalous thermal expansion believed to result from an invar effect were subtraction, as explained in [16], which discusses a series of Pu-Ga alloys. The Ce data are based on experiments on a Ce-Th alloy that undergoes the γ-α transition. The data used in this paper are given in the appendix.

In figure 1 we plot the quantity $k_B T_M/B\Omega$ versus the Grüneisen constant γ for 74 distinct

elements, some with several allotropes, for 81 entries. The plot shows a clear correlation between $k_B T_M / B\Omega$ and γ, but also many outliers, some of which are labeled. This plot expresses a connection between melting point and thermal expansion that has been known for a long time [21].

For further analysis, we divide the data into four groups according to crystal structure: BCC, FCC, HCP and *open structures*. On the basis of preliminary results, the "open" group is further divided into two subgroups, "1" and "2." Three elements with idiosyncratic planar structures are included with HCP: Sm, α-U and α-Pu. The subdivision of the "open" group and the reassignments to HCP are done on a provisional basis. Some of the structures considered are *not* the structures from which melting occurs. These structures are included as a practical matter, as data on the allotropes that *do* melt are not always available. In some cases, data are available for several allotropes, including the one that melts, and comparisons can be made, viz. Ce, Pu, Sn, P and C.

We use equation (1) as a starting point but use a more practical if less rigorous route for its evaluation. For S_{sol}, we use the Debye model. Wallace has discouraged the use of the measured Debye temperature for the evaluation of thermodynamic quantities, but we show in figure 2 that the correlation between the Θ_0 favored by Wallace and Θ_D is very strong. The only two obvious outliers are Fe and Ni. Figure 2 includes a plot of Θ_{el} calculated from the bulk modulus. We will use Θ_{el} later, but note for now that the points for Fe and Ni *do* fall properly on this curve, so we speculate that the neutron scattering data leading to the Θ_0 points for Fe and Ni are biased by magnetic effects. In that case, we may ignore the outliers and use the equivalence $\Theta_0 = 0.6 \; \Theta_D = e^{-1/3}\Theta_D$; the latter equivalence was suggested by Wallace. We now use the Debye model [22] to evaluate of S_{sol} arising from harmonic vibrations as $3\ln(Te^{4/3}/\Theta_D)$

In the solid we must include the effect of anharmonicity. If we recall that the difference in heat capacities $C_p - C_v$ is generally $\beta^2 B\Omega T/C_v$, it is easy to show that the anharmonic contribution to the entropy at high temperatures is $9\gamma^2 k_B T_M / B\Omega$.

For the liquid we follow Wallace with $S_L = S_{L,W}$. Now we can rewrite equation (1) as

$$\frac{3}{2}\ln\left(\frac{k_B Te}{\left(\frac{2\pi\hbar^2}{M\Omega^{\frac{2}{3}}}\right)}\right) - 3\ln\left(\frac{Te^{\frac{1}{3}}}{\Theta_D}\right) - 9\gamma^2\frac{k_B T}{B\Omega} = \Delta S - S_{corr} \tag{3}$$

To find a formula for the melting point, it is useful to replace the Debye temperature Θ_D by Θ_{el}, the corresponding quantity calculated from elastic constants, in equation (3), using the formula from elementary Debye theory [23]

$$1.3 k_B \Theta_D \approx k_B \Theta_{el} = \hbar\sqrt{\frac{B\Omega}{M}}\left(\frac{6\pi^2}{\Omega}\right)^{\frac{1}{3}} \tag{4}$$

to get an equation in the dimensionless variable $k_B T_M/B\Omega$. We have included a graph of Θ_{el} versus Θ_D in figure 2. A simple fitting procedure suggests that the equation can be improved by the prefactor 1.3, and we will allow this factor to be absorbed in the subsequent fitting procedure. It is known that a better formula for Θ_{el} can be obtained from a complete set of elastic constants so that the shear modes are included, but these data are not available in every case (especially high-temperature allotropes.) We have also ignored some small correction terms for extrapolating B and Ω from their values at measurement temperatures to those at the the melting point. When the replacement of Θ_D is made we find

$$-\frac{3}{2}\ln\left(\frac{k_B T}{B\Omega}\right) + \frac{3}{2}\ln\left(\frac{\left(6\pi^2\right)^{\frac{2}{3}}}{2\pi}\right) - \frac{5}{2} - 3\ln(1.3) - 9\gamma^2\frac{k_B T}{B\Omega} = \Delta S - S_{corr} \tag{5}$$

where the constant $3\ln(1.3)$ comes from equation (4). Collecting all the constants, we find

$$-\frac{3}{2}\ln\left(\frac{k_B T}{B\Omega}\right) - 9\gamma^2\frac{k_B T}{B\Omega} - \Delta S - 2.452 = -S_{corr} = a + b\gamma \tag{6}$$

It turns out that the term ($\Delta S - S_{corr}$) has a strong correlation with γ. Since ΔS is known for some (but not all) of the elements and also shows a linear correlation with γ we are able to find S_{corr}. All of these quantities are shown in figure 3, and the coefficient of the linear fit of $-S_{corr}$ versus γ are shown in Table 1.

Table 1: Fit parameters for $-S_{corr}$

	BCC	FCC	HCP	Open-1	Open-2
a	2.17±0.31	2.15±0.22	2.53±0.17	-0.88±0.44	-2.63±0.65
b	0.22±0.18	0.33±0.11	0.04±0.11	1.65±0.22	4.35±0.66

We find that S_{corr} is in the the range found by Wallace, between -2 and -3 for FCC, BCC and HCP, but spans a much wider range for the open structures. For FCC, BCC and HCP, the scatter in the $S_{liq,0}-S_{sol}$ data is enough that the correlation of S_{corr} with γ may not have much significance. For the open structures, the correlation is much stronger and cannot be ignored. When a and b from the entropy fits are used, equation 6 becomes a formula for the melting point. The calculated curves for $k_B T_M/B\Omega$ versus γ are plotted together with the data in figure 4, and the calculated melting points are plotted against the the observed melting points in figure 5.

The thermal atomic vibrational amplitude is related to $k_B T_M/B\Omega$ via [24]

$$\left\langle u^2 \right\rangle = \frac{3\hbar^2 T}{mk_B \Theta_{el}^2} \tag{7}$$

we have equation (4) for Θ, and the interatomic distance is $d_{atom} = 2(3\Omega/4\pi)^{1/3}$, so we get

$$relative\ amplitude = \frac{\sqrt{\left\langle u^2 \right\rangle}}{d_{atom}} = \frac{u_{avg}}{d_{atom}} = \sqrt{0.513\frac{k_B T_M}{B\Omega}} \tag{8}$$

The relative amplitude (RA) is plotted versus γ in figure 6. The RA is in the expected range for BCC, FCC and HCP over a wide range of γ, and the RA for Open-1 falls into that range for $\gamma \approx 2$. For

Open-2, the RA is consistently lower.

3. Discussion and Conclusions

The principal conclusion of this paper is that the Lindemann melting rule, that a solid melts when the vibrational amplitude reaches about 8% of the interatomic distance, follows from straightforward thermodynamic considerations for simple structures. There is no direct causal relationship between vibration and melting. The rule does not work as well for the "open-1" structures and does not work at all for the "open-2" structures. (Wallace's "anomalous" elements are all in the "Open-2" group.) Our discussion of the melting rule is based on the Debye model, which is expected to fail for complex structures [25]; we continue to use it for lack of an more accurate – yet still practical – procedure. Some of the data used in this paper pertain to crystalline phases stable at temperatures below the phase that actually melts. Despite these limitations, the melting points are predicated more or less successfully, albeit with significant errors; for example, the two allotropes of carbon, graphite and diamond, fall reasonably close to the ideal curves in figures 5 and 6. This shows that melting is essentially an atomic property.

For most of the elements, the anharmonic entropy of the solid is much less than the correlation entropy, as shown in figure 8. For these elements, we can say that the melting point is determined by a balance between the Debye entropy of the solid and the correlation entropy of the liquid. In exceptional cases, with high values of γ, the anharmonic entropy of the solid is involved in the balance. Thus the correlation entropy, a liquid state property, is found to depend on the Grüneisen constant γ, a solid state property. This connection between liquid and solid properties should be expected on the grounds that γ is a measure of the asymmetry of the interatomic potential about its minimum, and this asymmetry will also be important in the liquid state.

We consider the application of the Lindemann rule to the high melting carbide ZrC [26]. The ZrC structure is essentially the FCC structure filled up with interstitial carbon.. For ZrC, B is higher by

a factor 2.7, Ω is higher by a factor of 1.1 and γ is higher by 0.55 compared to elemental Zr. This suggests that the melting point of ZrC will be higher than that of Zr by a factor 2.3. Now ZrC melts at 2700K and Zr at 2100K, so the actual factor is 1.7. The level of precision is consistent with figures 5 and 6. Application of the Lindemann rule to ceramics with more complex structures is severely limited by the difficulties already encountered for open structures.

Two of the actinide considered in this paper have anomalously high values of the Grüneisen γ: γ-U and α-Pu. In view of the invar effect which operates in δ-phase Pu that that causes the uncorrected γ to be artificially low, we might expect that that and *anti*-invar effect, that would artificially enhance γ might be operative in these other actinide phases. Further experimental work on the thermal expansion of alloy-stabilized γ-U would be revealing. Further work is needed also on γ-Ce, for which an invar effect (*not anti*-invar) is predicted by the A-P model [27,28].

Questions about the melting points of the light actinides and rare earths were raised 40 years ago by Matthias et al. [29], who considered the minima near Ce and Pu shown in figure 1 and lamented the status of the contemporary theory of melting as "not even a satisfactory beginning," Smith and Kmetko published a composite phase diagram that emphasized the spectacular minimum in the actinides series [30] and has drawn much attention since. Now we can say that the melting point anomalies for the actinide series are determined by the elastic constants and volumes, which are themselves anomalous through their origins in correlated electron physics. In particular, the melting point of Pu is accounted for without any special assumptions about the liquid phase. Nothing further is involved.

Acknowledgments

Appendix: Data

Table A1: Atomic properties of selected elements

Structure	Name	Mass (g/mole)	$10^{-12}B$ (erg/cm³)	Volume (Å³)	Θ (K)	$10^6\alpha$ (K⁻¹)	γ	T_M (K)
BCC	Li	6.94	0.118	21.59	344	45	0.89	453
	Na	22.99	0.069	39.33	158	70.6	1.41	371
	K	39.1	0.032	75.35	91	83	1.46	337
	V	50.94	1.651	13.85	380	8.3	1.49	2160
	Cr	52	1.94	12.01	630	8.4	1.75	2130
	Fe	55.85	1.716	11.78	470	11.7	1.93	1808
	Rb	85.47	0.032	92.67	56	88.1	1.90	312
	Nb	92.91	1.736	18.01	275	7.07	1.67	2741
	Mo	95.94	2.779	15.59	450	4.98	1.75	2890
	Cs	132.91	0.021	117.88	38	97	1.74	302
	Ba	137.33	0.105	63.47	110	18.8	0.91	1002
	Eu	151.97	0.15	48.15	127	33.1	1.75	1095
	Ta	180.95	2.04	18.05	240	6.55	1.80	3269
	W	183.84	3.296	15.82	400	4.59	1.89	3680
	γ-U	238.03	1.14	22.05	270	22.5	4.12	1406
	ε-Pu	239	0.2	24.11	80	24.7	0.86	914
FCC	Al	26.98	0.736	16.61	428	23.1	2.26	934
	Ca	40.08	0.155	42.95	230	22.4	1.11	1112
	Ni	58.69	1.9	10.95	450	12.7	2.14	1726
	Cu	63.55	1.335	11.78	343	16.7	2.03	1356
	Sr	87.62	0.118	57.3	147	20	0.99	1042
	Rh	102.91	2.758	13.77	480	8.4	2.62	2239
	Pd	106.42	1.844	14.71	274	11.5	2.36	1825
	Ag	107.88	1.027	17.07	225	19.2	2.51	1235
	α-Ce	140.12	0.267	28.25	137	30	1.66	1072
	γ-Ce	140.12	0.244	34.74	137	8.5	0.53	1072
	Ir	192.22	3.62	14.13	420	6.63	2.71	2683
	Pt	195.08	2.838	15.11	240	8.95	2.87	2045
	Au	196.97	1.766	16.94	165	14.1	3.10	1338
	Pb	207.2	0.438	30.32	105	29	2.81	601
	Th	232.04	0.553	32.89	163	11.2	1.50	2023
	δ-Pu	239	0.289	25	125	9.5	0.50	914
HCP	Be	9.01	1.02	8.1	1440	11.5	1.75	1551
	Mg	24.3	0.361	23.23	400	25.6	1.70	922

		Sc	44.96	0.584	24.99	360	10	1.14	1814
		Ti	47.87	1.072	17.52	420	8.35	1.25	1933
		Co	58.93	1.952	11	445	12.4	2.15	1768
		Zn	65.39	0.61	15.23	327	29.7	2.12	693
		Y	88.9	0.373	35.42	280	12	1.20	1795
		Zr	91.22	0.85	23.29	291	5.78	0.87	2125
		Tc	98.91	3.03	14.29	351	8.06	2.71	2445
		Ru	101.07	3.271	13.57	600	9.36	3.65	2553
		Cd	112.41	0.477	21.59	209	30.6	2.34	594
		La	138.91	0.248	37.55	142	10.4	0.71	1194
		Pr	140.91	0.312	34.56	85	6.79	0.53	1204
		Nd	144.24	0.333	34.19	138	6.7	0.56	1294
		Pm	114.91	0.36	26.44	158	9	0.63	1441
		Sm	150.36	0.3	33.21	116	10.4	0.76	1350
		Gd	157.25	0.391	33.06	170	8.28	0.79	1586
		Tb	158.92	0.407	32.08	150	10.3	0.99	1629
		Dy	162.5	0.392	31.57	172	10	0.91	1685
		Ho	164.93	0.405	31.15	114	10.7	0.99	1747
		Er	167.26	0.42	30.65	134	12.3	1.16	1802
		Tm	168.93	0.405	30.11	127	13.3	1.19	1818
		Yb	173.04	0.135	41.27	120	24.96	1.02	1097
		Lu	174.98	0.419	29.54	210	8.12	0.75	1936
		Hf	178.49	1.11	22.28	252	6.01	1.12	2503
		Re	186.21	3.79	14.72	430	6.63	2.96	3453
		Os	190.23	4.26	14.04	500	4.7	2.33	3327
		Tl	204.38	0.366	28.65	78.5	29.4	2.24	577
		α-U	238.03	1.35	20.87	207	12.6	2.63	1406
		α-Pu	239	0.546	20.01	160	55	4.42	914
Open-1		B	10.81	1.82	7.67	1315	8.3	1.87	2573
	C (graphite)		12.01	0.345	9.02	402	3.8	0.09	3830
	C (diamond)		12.01	5.56	8.74	2230	1.19	2.53	3830
	P (red)		30.97	0.196	21.89	325	66.5	2.19	317
	· P (white)		30.97	0.048	23.19	193	124.5	1.03	317
	S (rhomb)		32.07	0.182	27.18	200	64.1	2.35	386
		α-Mn	54.94	0.608	12.27	410	22.6	1.34	1517
		Se	78.96	0.093	27.38	90	36.9	0.68	490
		In	114.82	0.418	26.09	108	31.4	2.50	429
		α-Sn	118.71	0.553	34.29	236	21.2	3.00	505
		Hg	200.59	0.288	24.6	71.9	61	3.15	234

Open-2	Si	28.08	1.008	20.03	645	3.07	0.56	1683
	Ga	69.72	0.58	19.61	320	18.1	1.58	303
	Ge	72.61	0.787	22.66	374	5.75	0.80	1211
	As	74.92	0.402	21.53	282	4.28	0.28	1090
	β-Sn	118.71	1.13	26.98	196	5.3	1.20	505
	Sb	112.76	0.39	27.99	211	10.9	0.88	904
	Te	127.8	0.235	34.02	153	16.77	0.98	723
	Bi	208.98	0.321	35.62	119	13.41	1.12	545

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Figure Captions

Figure 1. Periodic table of melting points.

Figure 2. $k_B T_M/B\Omega$ versus Grüneisen γ. The line $k_B T_M/B\Omega = 0.3e^{-0.5\gamma}$ is shown as a guide, and a few outlying points are labeled.

Figure 3. Wallace's entropy Θ_0 and the elastic Θ_{el} (from equation 4) plotted versus the Debye Θ_D.

Figure 4. Entropy difference S_{S-T}-S_{Debye}-S_{Anhar}, measured entropy of melting ΔS_{meas}, and -S_{corr} from equation 6 plotted versus Grüneisen γ for different structural groups.

Figure 5. Fitted $k_B T_M/B\Omega$ versus Grüneisen γ for different structural groups.

Figure 6. Calculated T_M versus measured T_M for different structural groups.

Figure 7. Calculated relative thermal atomic vibration amplitudes (RAs) from equation 8 plotted versus Grüneisen γ for different structure groups.

Figure 8. Ratio of solid anharmonic entropy to liquid correlation entropy, $S_{anhar}/(-S_{corr})$ plotted versus Grüneisen γ for different structure groups.
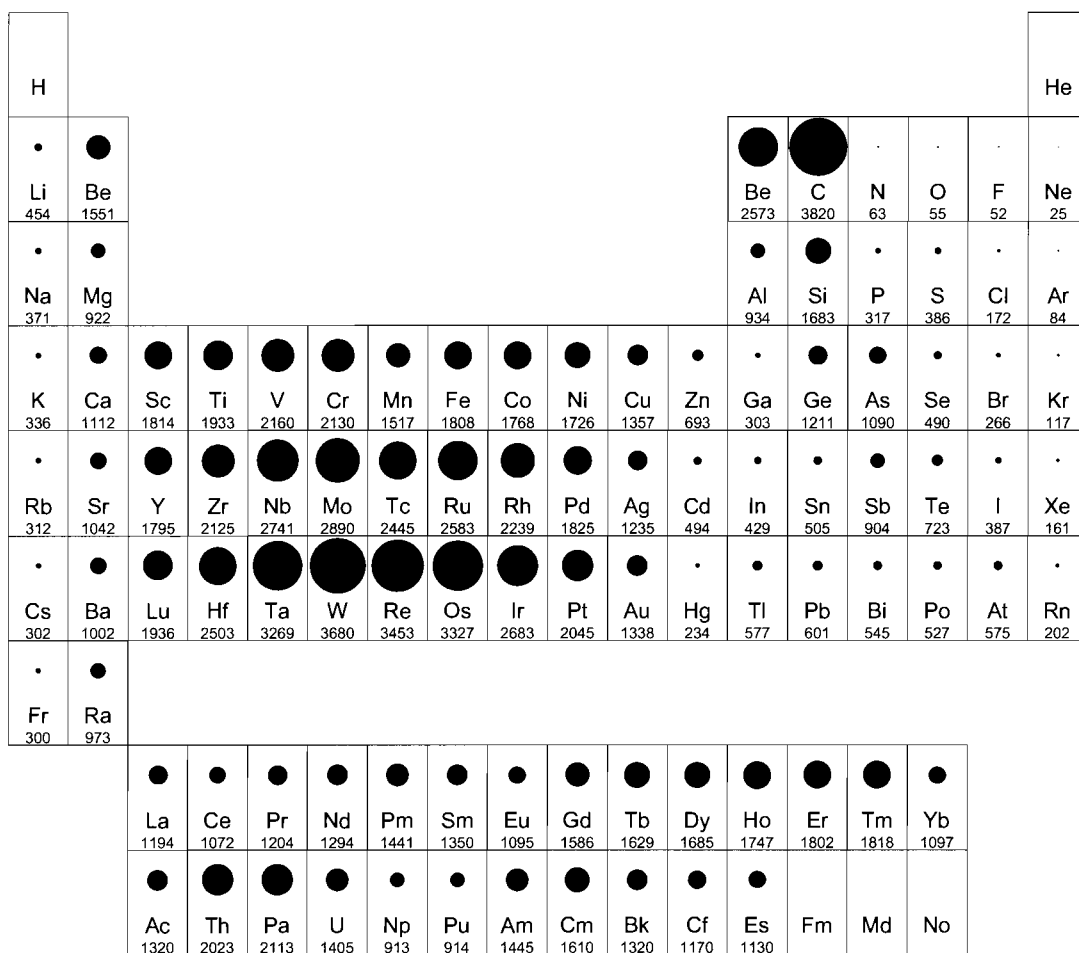
H																	He
Li 454	Be 1551											B 2573	C 3820	N 63	O 55	F 52	Ne 25
Na 371	Mg 922											Al 934	Si 1683	P 317	S 386	Cl 172	Ar 84
K 336	Ca 1112	Sc 1814	Ti 1933	V 2160	Cr 2130	Mn 1517	Fe 1808	Co 1768	Ni 1726	Cu 1357	Zn 693	Ga 303	Ge 1211	As 1090	Se 490	Br 266	Kr 117
Rb 312	Sr 1042	Y 1795	Zr 2125	Nb 2741	Mo 2890	Tc 2445	Ru 2583	Rh 2239	Pd 1825	Ag 1235	Cd 494	In 429	Sn 505	Sb 904	Te 723	I 387	Xe 161
Cs 302	Ba 1002	Lu 1936	Hf 2503	Ta 3269	W 3680	Re 3453	Os 3327	Ir 2683	Pt 2045	Au 1338	Hg 234	Tl 577	Pb 601	Bi 545	Po 527	At 575	Rn 202
Fr 300	Ra 973																

La 1194	Ce 1072	Pr 1204	Nd 1294	Pm 1441	Sm 1350	Eu 1095	Gd 1586	Tb 1629	Dy 1685	Ho 1747	Er 1802	Tm 1818	Yb 1097
Ac 1320	Th 2023	Pa 2113	U 1405	Np 913	Pu 914	Am 1445	Cm 1610	Bk 1320	Cf 1170	Es 1130	Fm	Md	No

Figure 1: Periodic table of melting points.

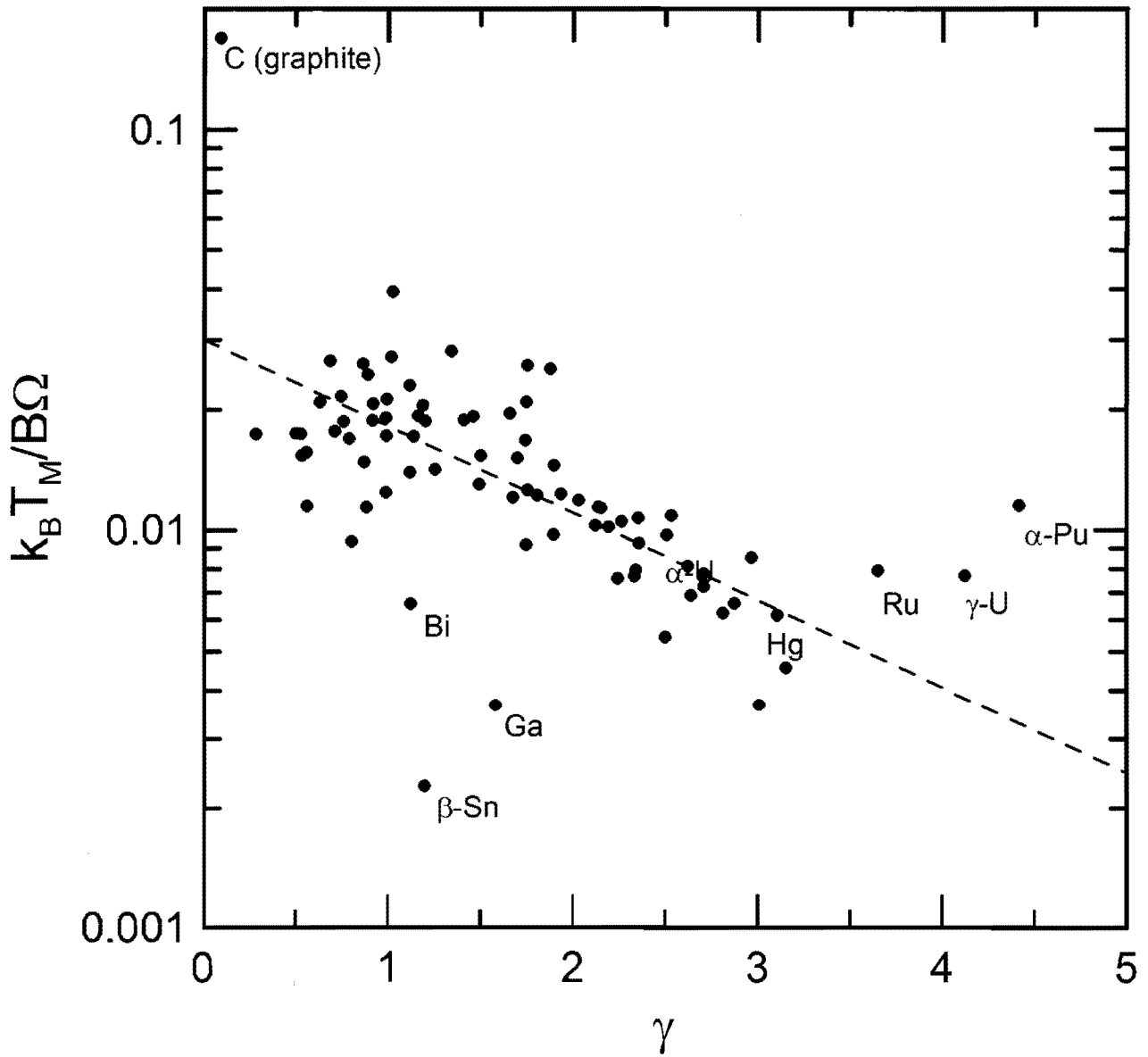*Figure 2:* $k_B T_M/B\Omega$ *versus Grüneisen* γ. *The line* $k_B T_M/B\Omega = 0.3e^{-0.5\gamma}$ *is shown as a guide, and a few outlying points are labeled.*
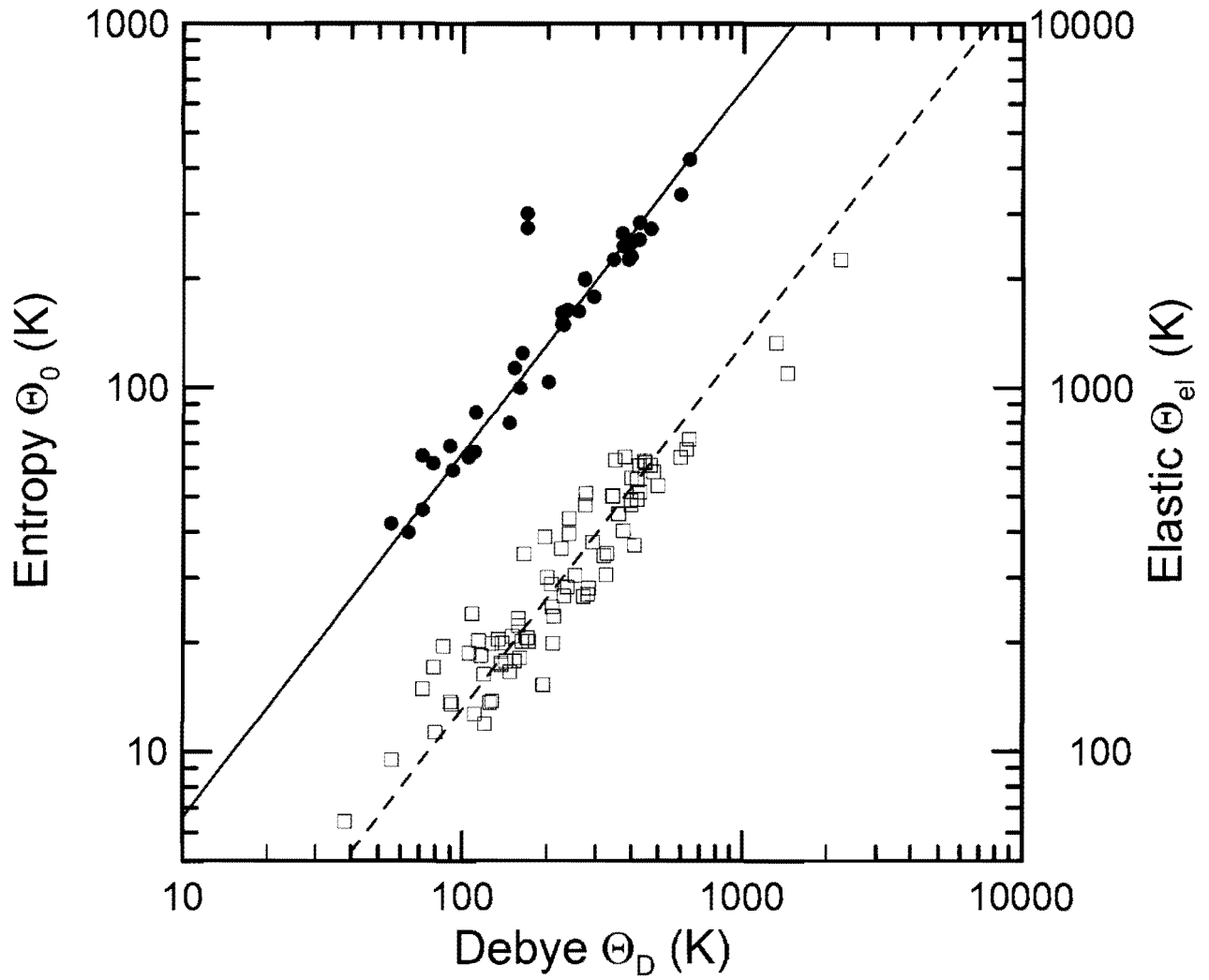
Figure 3: Wallace's entropy Θ_0 and the elastic Θ_{el} from equation 4 plotted versus the Debye Θ_D.
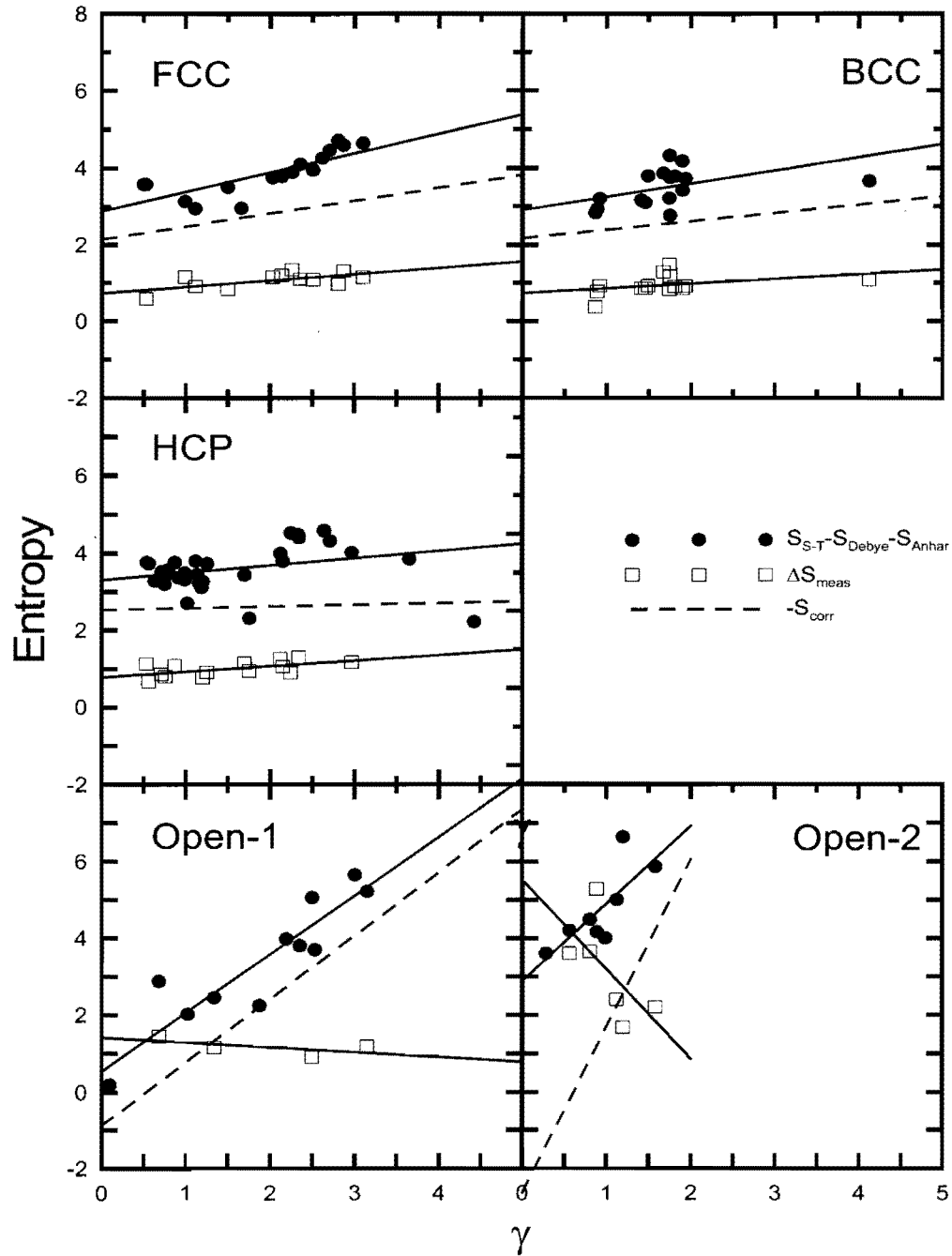
Figure 4: Entropy difference S_{S-T}-S_{Debye}-S_{Anhar} measured entropy of melting ΔS_{meas}, and -S_{corr} from equation 6 plotted versus Grüneisen γ for different structural groups.
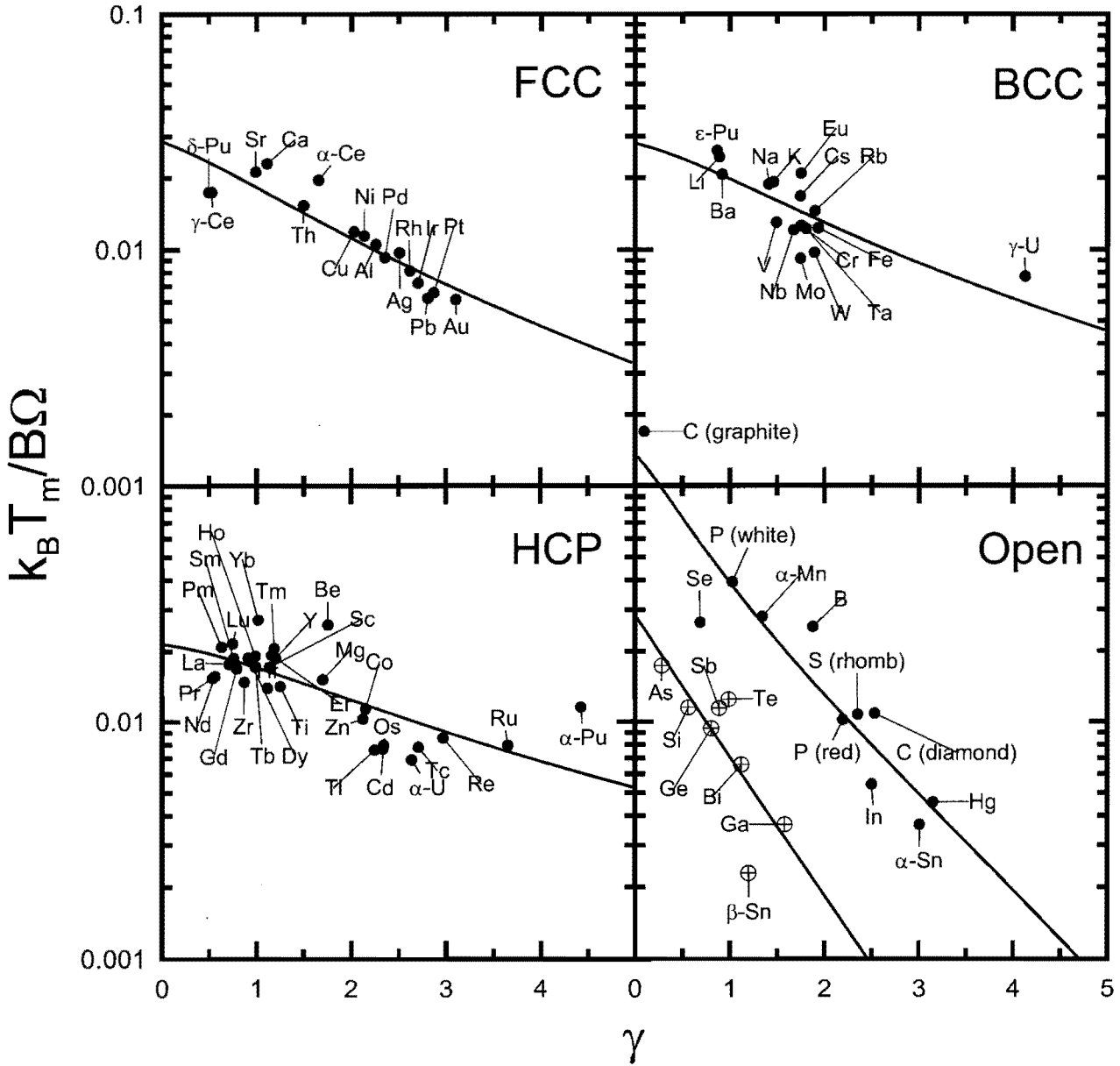
Figure 5: Fitted $k_B T_M/B\Omega$ versus Grüneisen γ for different structural groups.
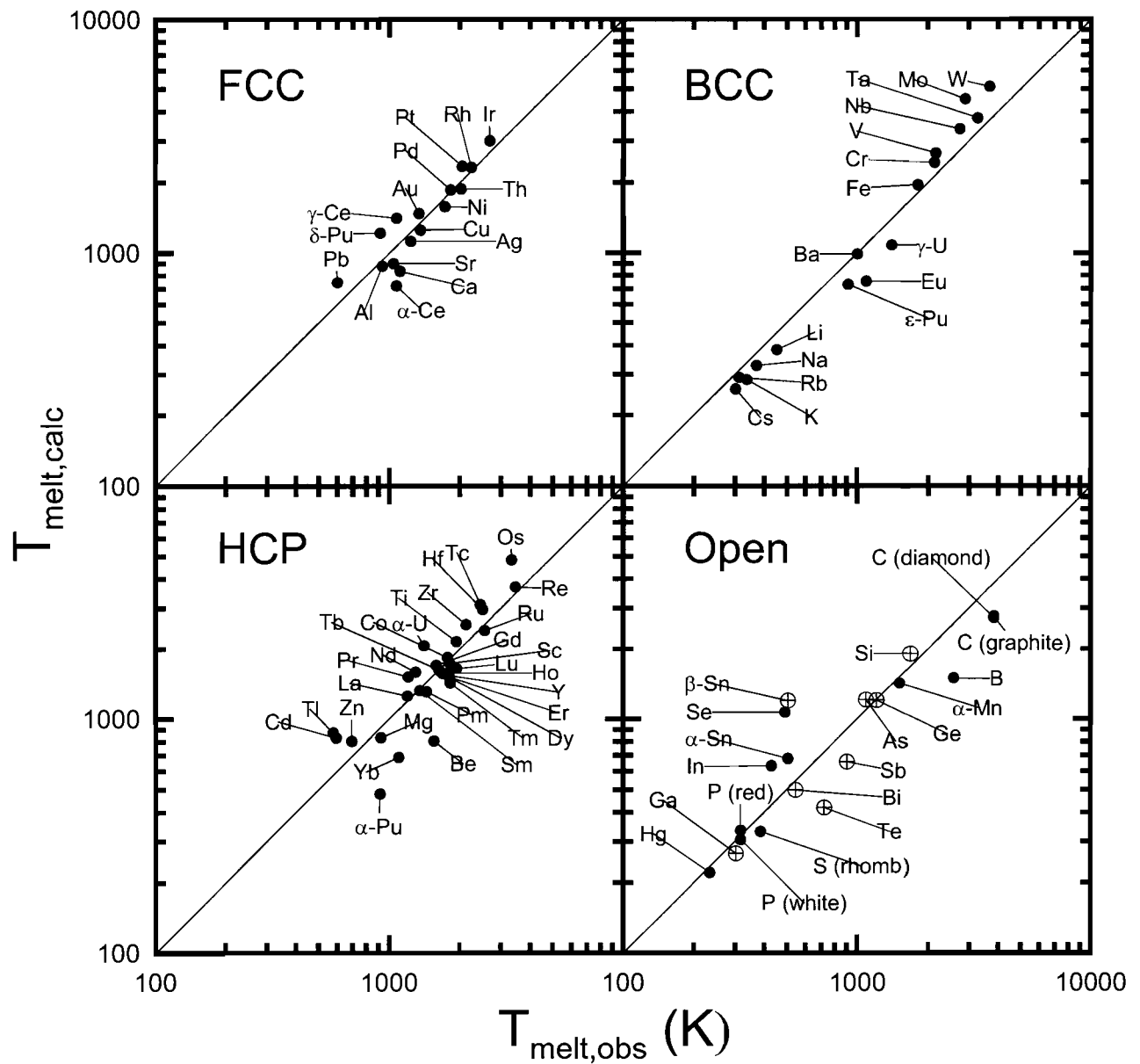
Figure 6: Calculated T_M versus measured T_M for different structural groups.
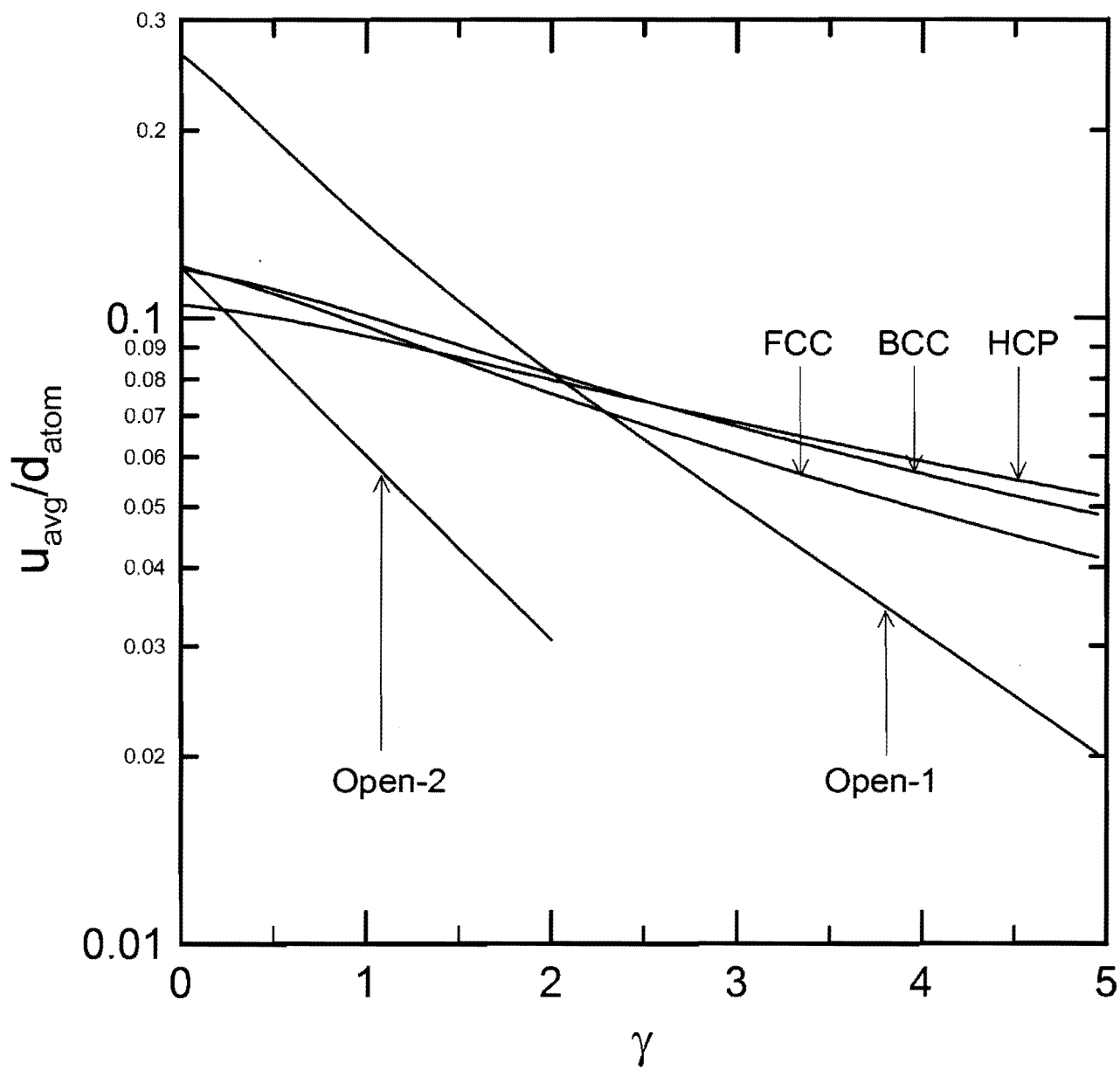
Figure 7: Calculated relative thermal atomic vibration amplitudes (RAs) from equation 7 plotted versus Grüneisen γ for different structure groups.

Figure 8: Ratio of solid anharmonic entropy to liquid correlation entropy, $S_{anhar}/(-S_{corr})$ plotted versus Grüneisen γ for different structure groups.