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Tantalum Shear Modulus from Homogenization of Single Crystal Data

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Elastic constants for tantalum single crystals have been calculated by Orlikowski, et al. [1] for a broad range of temperatures and pressures. These moduli can be utilized directly in continuum crystal simulations or dislocation dynamics calculations where the individual grains of the polycrystalline material are explicitly represented. For simulations on a larger size scale, the volume of material represented by the quadrature points of the simulation codes includes many grains, and average moduli are needed. Analytic bounding and averaging schemes exist, but since these do not account for nonuniform stress and strain within the interacting grains, the upper and lower bounds tend to diverge as the crystal anisotropy increases. Local deformation and stress equilibrium accommodate the anisotropic response of the individual grains.

One method of including grain interactions in shear modulus averaging calculations is through a highly-descretized finite element model of a polycrystal volume. This virtual test sample (VTS) can be probed to determine the average response of the polycrystal. The desire to obtain isotropic moduli imposes attributes on the VTS. The grains should be equiax and the crystal orientation distribution function should be random. For these simulations, a cube, 300 μm on a side, was discretized with 1 million finite elements on a regular rectangular mesh. The mesh was seeded with 1000 grains generated using a constrained-random placement algorithm, Figure 1. Since the orientations were simply painted in the mesh, the grain boundaries are irregular. The orientation distribution function is shown as pole figure in Figure 2. It has the appearance of being random. Analysis of the simulation results will be used to determine if the randomness of the texture and number of grains are adequate.

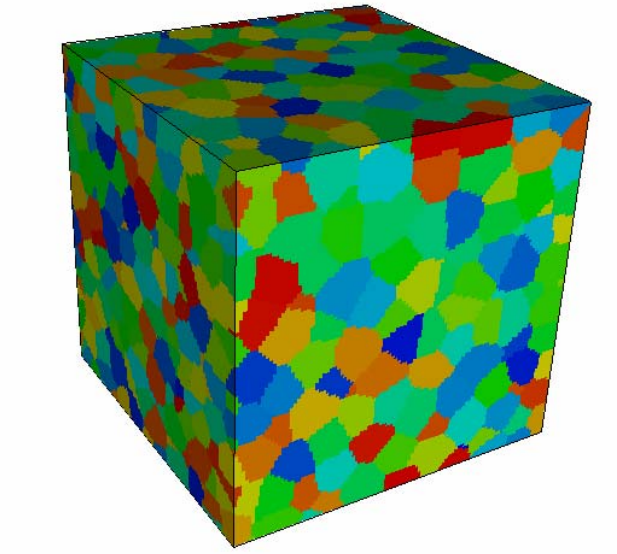

Figure 1 Polycrystal Virtual Test Sample with 1000 grains. Color indicates grain orientation.

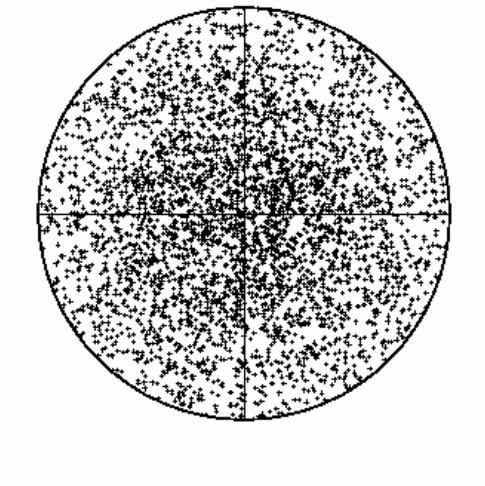

Figure 2 (111) pole figure showing the crystal orientation distribution function

Boundary conditions consistent with pure shear deformation are applied to all nodes on the exterior of the cube. The simulations were run using the implicit capability in ALE3D on 128 processors of ASC-UP. To gage and reduce the effects of anisotropy in the VTS, six distinct pure shear modes are probed and averaged: $\varepsilon_{12}; \varepsilon_{23}; \varepsilon_{31}; \varepsilon_{11}-\varepsilon_{22};\ \varepsilon_{22}-\varepsilon_{33};$ and $\varepsilon_{33}-\varepsilon_{11}$. Each set of six simulations is conducted using single crystal moduli at the specified temperature and pressure. Temperatures examined range from 0K to 4000K and pressures from 0 to 1000 GPa. (A partial listing of the tables from Orlikowski, et al. [1] is given in Appendix A.) The material remains elastic during the simulations. The isotropic shear modulus, *G*, is calculated by equating the calculated elastic energy per unit volume (*E*) to an ideal elastic solid at the same strain.

$$E = G\left(\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2 + 2\varepsilon_{12}^2 + 2\varepsilon_{23}^2 + 2\varepsilon_{31}^2\right)$$

Only one or two or the strains are nonzero for each run, depending upon which of the six shear modes is being analyzed.

Results

The averages of the six modulus calculations over the range of temperature and pressure conditions are presented in Table 1. The results exhibit a roughly linear dependence in both temperature and pressure, with the pressure effects being dominant. The trend is shown in Figure 3. Examination of the temperature dependence reveals a shift in slope with temperature at 300K. This is evident in the single crystal moduli input to the VTS simulations and corresponds to the Debye temperature[1].

A plot of the standard deviation among the six runs at each condition is given in Figure 4. The variation is below 1% over the range of pressures and temperatures, indicating that the VTS yields results nearly independent of orientation. It is inferred that the randomness in crystal orientation distribution and grain shape are adequate for these simulations.

Table 1: Shear modulus, in GPa, calculated from finite element homogenization of a VTS. Temperature in K varies down the columns. Pressure in GPa varies across the rows.

P(GPa) **T**(k)	0	100	200	300	400	500	600	700	800	900	1000
0	71.2	148.1	225.8	308.5	394.6	481.9	569.9	658.1	745.9	832.3	919.8
100	68.8	143.3	223.2	307.7	394.0	480.7	567.7	655.2	743.5	832.8	925.0
200	66.8	139.5	221.1	306.8	393.4	479.5	565.6	652.5	741.1	832.5	928.3
300	65.4	137.3	219.7	306.0	392.4	478.0	563.4	649.7	738.2	830.2	927.3
600	62.9	135.6	217.4	302.6	388.0	472.8	557.5	642.9	730.3	820.8	915.9
900	60.8	135.0	215.7	299.6	384.1	468.4	552.6	637.6	724.0	812.8	905.2
1200	58.5	133.7	214.7	298.2	382.0	465.4	548.7	632.4	717.5	804.6	895.0
1500	55.9	131.9	214.3	298.3	381.5	463.7	545.2	627.0	710.2	795.9	885.1
1800	53.4	129.9	214.1	298.8	381.5	462.2	541.9	621.6	702.8	787.2	875.8
2100	50.9	128.1	213.6	298.7	380.8	460.3	538.2	616.2	695.8	779.0	867.1
2400	48.4	126.4	212.6	297.5	378.8	457.2	533.9	610.6	689.1	771.5	859.1
2700	46.1	124.8	211.3	295.8	376.1	453.0	528.4	603.9	681.5	763.6	851.4
3000	43.9	123.3	210.1	293.7	372.5	447.7	521.3	595.5	672.5	754.8	843.8
3500	41.3	120.8	207.8	290.1	366.1	437.9	508.3	579.9	655.6	738.7	830.9
4000	38.5	118.1	205.3	286.5	360.0	428.5	495.6	564.6	638.9	722.3	817.3

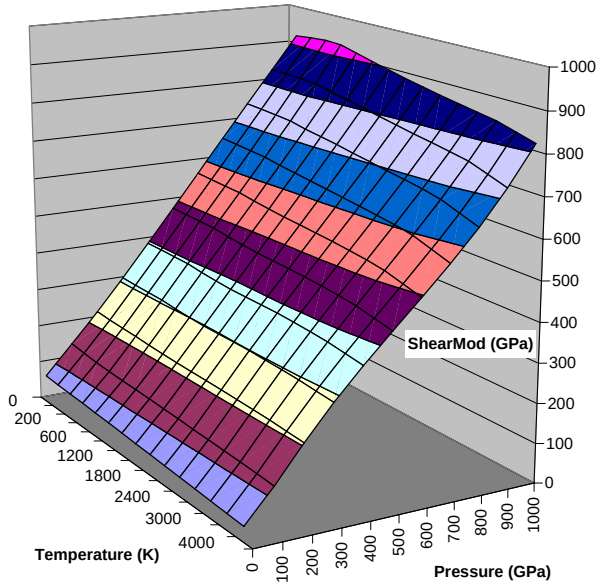

Figure 3 Isotropic shear modulus as a function of temperature and pressure

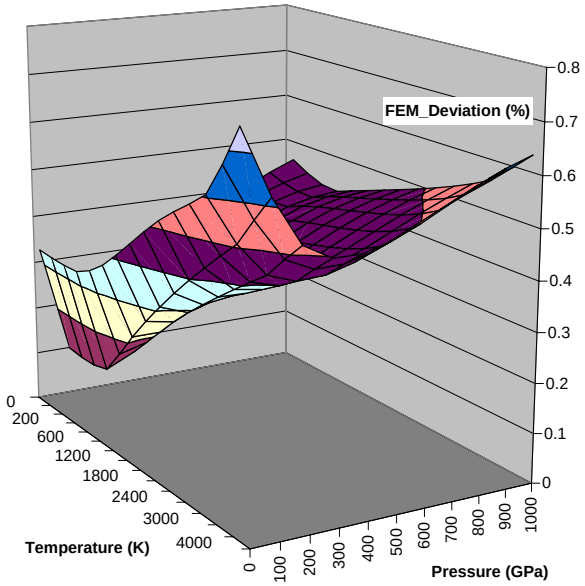

Figure 4 Standard deviation among the six modulus calculations

In the temperature range from 300K-3000K the shear modulus can be approximated fairly well by a bi-quadratic function.

$$G = A + A_T T + A_{T^2} T^2 + \left(A_P + A_{TP} T + A_{T^2P} T^2\right) P + \left(A_{P^2} + A_{TP^2} T + A_{T^2P^2} T^2\right) P^2$$

A = 67.575 GPa	A_T = -7.698E-03 GPa	A_{T2} = 3.282E-07 GPa
A_P = 0.770	A_{TP} = 2.629E-05	A_{T2P} = -3.459E-09
A_{P2} = 1.329E-04 GPa^{-1}	A_{TP2} = -1.060E-07 GPa^{-1}	A_{T2P2} = 1.864E-11 GPa^{-1}

This parameterization was obtained by first creating a least squares fit over the range of pressures at constant temperature, and then calculating a fit for those coefficients over a 300K-3000K temperature range. The 0 pressure data were entered into the fitting equation multiple times to reduce the magnitude of the error at low pressures. A shift of a few GPa is a significant fraction of the modulus at low pressures but not at high pressures. The quality of this fit is shown by the relative error plotted in Figure 5. The deviation between the VTS results and the bi-quadratic fit is less than 5% over most of the range, with the most severe deviations being at lower pressures. If this same fit is extended over the full range of the VTS results, the deviation is larger, Figure 6. The bi-quadratic fit provides a reasonable and smooth parameterization of the shear modulus. The tabular representation can used for closer correspondence to the first principles calculations.

It is instructive to compare the shear modulus calculated by VTS homogenization of first principles single crystal moduli to the Steinberg-Guinan (SG) [2] shear modulus model. The SG representation includes a density ratio term, so the modulus calculations also involve the Equation of State (EOS). Here the "Blue Book"[2] values for the modulus and Gruneisen EOS are employed. The modulus and EOS expressions are given by:

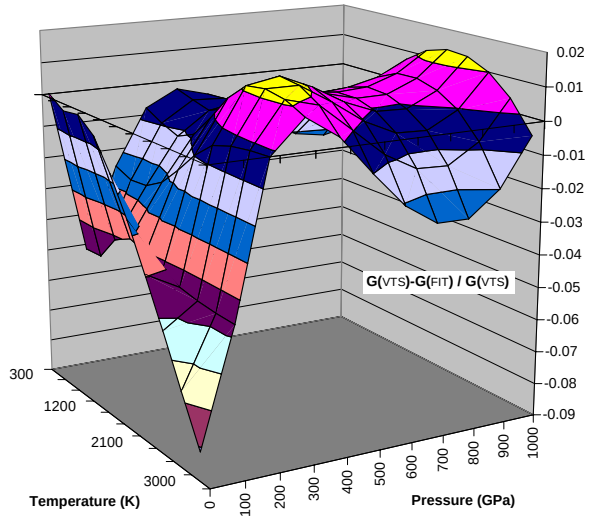

Figure 5 Deviation of bi-quadratic fit compared to VTS results from 300K-3000K

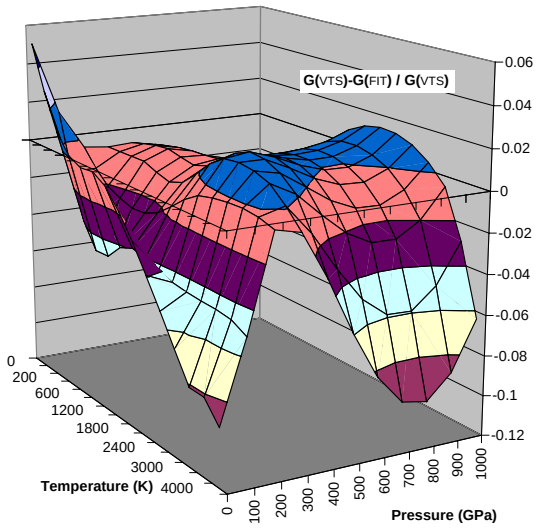

Figure 6 Deviation of bi-quadratic fit compared to VTS results from 0K-4000K

$$G_{(GPa)} = 69\left[1 + 0.0145P\left(\frac{\rho_0}{\rho}\right)^{1/3} - 0.00013(T-300)\right]$$

.

$$P_{(GPa)} = \frac{194.07\mu\left(1+0.165\mu-0.21\mu^2\right)}{(1-0.2\mu)^2} + (1.67+0.42\mu)\,0.002288\,(T-300), \qquad \mu = \frac{\rho}{\rho_0} - 1$$

For a given pressure and temperature, the EOS is inverted to determine the density ratio for modulus calculation. The Gruneisen fit has a singularity at high compressions, so the density ratio use in the SG shear modulus calculations is set to 2.3 for pressures greater than 500 GPa.

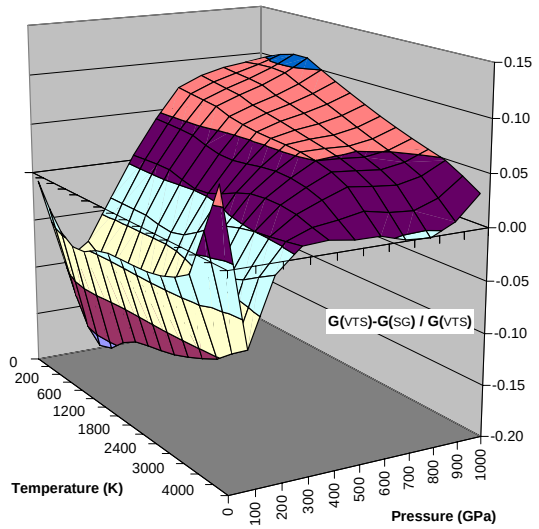

Figure 7 Deviation of the SG shear modulus from the VTS calculations

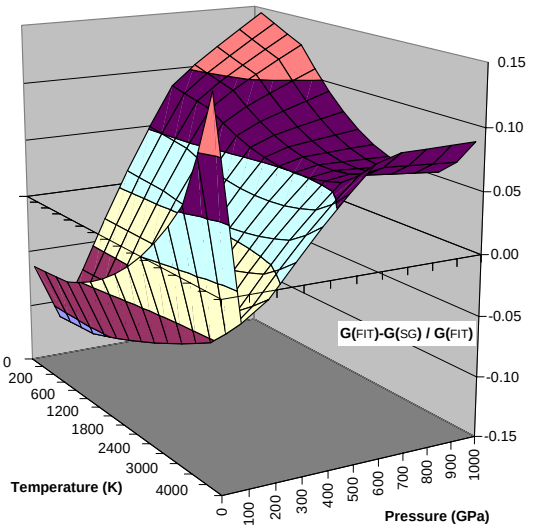

Figure 8 Deviation of the SG shear modulus from the biquadratic fit to the VTS results

Using the 0 GPa-300 K result as a comparison point, the VTS simulations give 65.4 GPa whereas the value from the SG model is 69 GPa. This is roughly a 5% difference between a first principles calculation and the corresponding experimental value. This lower value is consistent with the C` and C_{44} values being slightly lower than experimental data in Orlikowski et al. [1]. The deviations between the VTS results and SG relation over the entire temperature and pressure range are given in Figure 7 and the biquadratic fit is compared with the SG shear modulus in Figure 8. The differences range to approximately 15% in both comparisons. This suggests that the SG shear modulus model for tantalum is not unreasonable when applied over a broad range of temperatures and pressures.

Acknowledgements: The moduli used as the basis for these calculations and included in the appendix were graciously supplied by D. Orlikowski, P. Söderlind and J.A. Moriarty. The simulations were supported by the ASC Physics and Engineering Models program. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

References:

[1] D. Orlikowski, P. Söderlind and J.A. Moriarty, "First-principles thermoelasticty of transition metals at high pressure: Tantalum prototype in the quasiharmonic limit," *Phys. Rev. B*, **74**, 2006, 054109.

[2] D.J. Steinberg, "Equation of state and strength properties of selected materials," Lawrence Livermore National Laboratory, UCRL-MA-106439.

Appendix A: Partial listing of pressure and temperature dependent crystal moduli, in GPa, obtained from Orlikowski et al. [1]

	T=0			T=100			T=200		
P(GPa)	C11	C12	C44	C11	C12	C44	C11	C12	C44
0.0	271.3	171.5	88.9	264.6	167.9	85.7	258.8	164.8	83.1
20.4	364.7	227.7	102.7	354.9	223.0	97.9	346.5	219.2	94.2
40.8	454.9	282.8	116.7	443.4	277.7	111.0	433.5	273.5	106.7
61.2	542.6	337.2	130.9	530.4	332.1	124.9	519.9	328.0	120.4
81.6	628.4	391.1	145.6	616.3	386.4	139.7	605.7	382.7	135.4
102.0	712.7	444.7	160.9	701.1	440.8	155.4	690.8	437.6	151.4
122.4	795.7	498.3	176.9	785.0	495.2	172.0	775.4	492.7	168.5
142.9	877.8	551.9	193.5	868.2	549.8	189.4	859.3	548.1	186.5
163.3	959.1	605.6	210.9	950.6	604.5	207.6	942.7	603.6	205.4
183.7	1039.8	659.6	229.1	1032.4	659.5	226.6	1025.4	659.4	225.1
204.1	1119.9	713.8	247.9	1113.7	714.7	246.3	1107.5	715.4	245.5
224.5	1199.7	768.2	267.5	1194.4	770.1	266.7	1189.0	771.5	266.5
244.9	1279.0	822.9	287.7	1274.6	825.6	287.7	1269.9	827.8	288.0
265.3	1358.0	877.9	308.6	1354.3	881.3	309.2	1350.1	884.1	310.1
285.7	1436.7	933.1	330.1	1433.5	937.2	331.3	1429.8	940.5	332.6
306.1	1515.1	988.6	352.1	1512.3	993.2	353.9	1508.9	997.0	355.6
326.5	1593.2	1044.3	374.7	1590.6	1049.3	376.8	1587.5	1053.5	378.8
346.9	1671.0	1100.2	397.7	1668.5	1105.5	400.2	1665.5	1110.0	402.4
367.3	1748.6	1156.3	421.1	1746.0	1161.8	423.9	1742.9	1166.4	426.3
387.8	1825.9	1212.6	445.0	1823.1	1218.2	447.9	1820.0	1222.9	450.5
408.2	1903.0	1269.1	469.2	1899.8	1274.6	472.3	1896.5	1279.3	474.8
428.6	1979.9	1325.8	493.8	1976.3	1331.1	496.9	1972.7	1335.6	499.4
449.0	2056.7	1382.7	518.7	2052.5	1387.6	521.7	2048.5	1391.9	524.2
469.4	2133.3	1439.8	543.9	2128.4	1444.1	546.7	2124.0	1448.1	549.1
489.8	2209.8	1497.1	569.3	2204.1	1500.8	572.0	2199.1	1504.3	574.1
510.2	2286.3	1554.5	595.1	2279.7	1557.4	597.4	2274.1	1560.4	599.4
530.6	2362.7	1612.2	621.0	2355.2	1614.2	623.1	2348.8	1616.4	624.7
551.0	2439.1	1670.2	647.3	2430.5	1671.0	648.9	2423.4	1672.4	650.2
571.4	2515.5	1728.3	673.7	2505.8	1727.8	674.9	2497.9	1728.4	675.8
591.8	2592.1	1786.7	700.3	2581.1	1784.8	701.0	2572.3	1784.3	701.5
612.2	2668.6	1845.3	727.1	2656.5	1841.8	727.2	2646.7	1840.2	727.3
632.7	2745.3	1904.1	754.0	2731.8	1898.9	753.6	2721.1	1896.0	753.2
653.1	2822.1	1963.2	781.2	2807.3	1956.1	780.1	2795.5	1951.8	779.2
673.5	2899.0	2022.4	808.4	2882.8	2013.3	806.7	2870.0	2007.5	805.3
693.9	2976.1	2081.9	835.7	2958.4	2070.6	833.4	2944.6	2063.2	831.5
714.3	3053.2	2141.6	863.1	3034.2	2127.9	860.1	3019.4	2118.8	857.7
734.7	3130.4	2201.4	890.6	3110.1	2185.3	887.0	3094.2	2174.3	884.1
755.1	3207.7	2261.4	918.1	3186.1	2242.8	913.8	3169.3	2229.8	910.5
775.5	3285.0	2321.5	945.6	3262.3	2300.2	940.7	3244.5	2285.2	936.9
795.9	3362.4	2381.8	973.1	3338.6	2357.7	967.6	3320.0	2340.6	963.4
816.3	3439.8	2442.2	1000.5	3415.1	2415.1	994.6	3395.7	2395.8	989.9
836.7	3517.2	2502.6	1027.9	3491.8	2472.6	1021.5	3471.7	2450.9	1016.5
857.1	3594.7	2563.2	1055.2	3568.6	2530.0	1048.4	3547.9	2506.0	1043.2
877.6	3672.4	2623.9	1082.5	3645.8	2587.5	1075.4	3624.6	2561.0	1069.9
898.0	3750.1	2684.7	1109.7	3723.2	2645.1	1102.3	3701.6	2616.0	1096.7
918.4	3828.2	2745.8	1137.0	3801.0	2702.7	1129.4	3779.1	2670.9	1123.5
938.8	3906.8	2807.2	1164.3	3879.3	2760.6	1156.5	3857.2	2725.9	1150.5
959.2	3986.0	2869.1	1191.7	3958.3	2818.7	1183.7	3935.8	2781.1	1177.7
979.6	4066.3	2931.7	1219.5	4038.1	2877.2	1211.2	4015.2	2836.4	1205.1
1000.0	4147.9	2995.1	1247.7	4119.1	2936.3	1239.1	4095.5	2892.2	1232.8

	T=300			T=600			T=900		
P(GPa)	C11	C12	C44	C11	C12	C44	C11	C12	C44
0.0	254.3	162.5	81.5	244.3	157.7	79.3	234.6	153.5	77.9
20.4	340.4	216.7	92.2	329.0	213.4	91.8	318.5	210.4	92.7
40.8	426.4	271.1	104.6	413.8	268.9	105.6	402.3	266.9	108.0
61.2	512.3	325.8	118.5	498.5	324.4	120.4	486.0	323.0	123.9
81.6	597.9	380.8	133.6	583.1	379.9	136.3	569.6	378.9	140.6
102.0	683.1	436.0	150.0	667.4	435.5	153.2	653.1	434.8	157.8
122.4	767.8	491.5	167.4	751.4	491.4	170.9	736.3	490.8	175.8
142.9	852.0	547.3	185.8	835.1	547.3	189.4	819.2	546.9	194.4
163.3	935.7	603.3	205.0	918.2	603.5	208.8	901.9	603.1	213.6
183.7	1018.8	659.5	225.1	1001.0	659.8	228.7	984.1	659.6	233.4
204.1	1101.3	715.8	245.8	1083.1	716.3	249.3	1066.1	716.2	253.7
224.5	1183.1	772.3	267.1	1164.8	772.9	270.5	1147.6	773.0	274.5
244.9	1264.3	828.9	288.9	1245.8	829.7	292.2	1228.7	830.0	295.9
265.3	1344.9	885.6	311.2	1326.3	886.5	314.3	1309.3	887.2	317.6
285.7	1424.8	942.3	334.0	1406.3	943.4	336.8	1389.6	944.4	339.7
306.1	1504.0	999.0	357.0	1485.6	1000.4	359.6	1469.4	1001.8	362.3
326.5	1582.7	1055.7	380.4	1564.5	1057.4	382.8	1548.7	1059.3	385.1
346.9	1660.8	1112.3	404.1	1642.8	1114.3	406.2	1627.6	1116.8	408.2
367.3	1738.3	1168.9	428.1	1720.6	1171.3	429.9	1706.1	1174.4	431.6
387.8	1815.3	1225.4	452.2	1797.9	1228.2	453.9	1784.1	1231.9	455.3
408.2	1891.8	1281.9	476.5	1874.7	1285.0	478.0	1861.8	1289.4	479.1
428.6	1967.8	1338.2	501.0	1951.1	1341.8	502.3	1939.0	1346.9	503.2
449.0	2043.5	1394.5	525.7	2027.2	1398.5	526.8	2015.9	1404.4	527.5
469.4	2118.8	1450.6	550.5	2102.9	1455.1	551.4	2092.5	1461.7	551.9
489.8	2193.8	1506.6	575.4	2178.2	1511.6	576.1	2168.7	1519.0	576.5
510.2	2268.4	1562.6	600.5	2253.3	1568.0	601.0	2244.6	1576.2	601.2
530.6	2342.9	1618.4	625.6	2328.1	1624.4	626.0	2320.3	1633.3	626.1
551.0	2417.2	1674.1	650.9	2402.7	1680.6	651.1	2395.7	1690.2	651.1
571.4	2491.3	1729.8	676.3	2477.2	1736.7	676.4	2470.9	1747.1	676.3
591.8	2565.3	1785.3	701.7	2551.5	1792.7	701.7	2545.9	1803.8	701.6
612.2	2639.3	1840.8	727.3	2625.7	1848.6	727.1	2620.6	1860.4	726.9
632.7	2713.2	1896.1	752.9	2699.8	1904.4	752.7	2695.3	1916.8	752.4
653.1	2787.2	1951.3	778.7	2773.8	1960.0	778.3	2769.8	1973.0	778.1
673.5	2861.2	2006.5	804.5	2847.9	2015.5	804.0	2844.2	2029.1	803.7
693.9	2935.3	2061.5	830.4	2921.9	2070.9	829.8	2918.4	2085.0	829.5
714.3	3009.5	2116.5	856.4	2996.0	2126.1	855.7	2992.6	2140.6	855.4
734.7	3083.9	2171.3	882.4	3070.2	2181.1	881.7	3066.7	2196.0	881.3
755.1	3158.4	2226.0	908.5	3144.5	2236.0	907.7	3140.8	2251.1	907.3
775.5	3233.2	2280.6	934.8	3218.8	2290.7	933.8	3214.8	2306.0	933.3
795.9	3308.2	2335.1	961.0	3293.4	2345.2	959.9	3288.8	2360.5	959.3
816.3	3383.5	2389.4	987.4	3368.1	2399.5	986.1	3362.8	2414.7	985.4
836.7	3459.1	2443.6	1013.8	3443.0	2453.5	1012.3	3436.7	2468.6	1011.4
857.1	3535.0	2497.7	1040.3	3518.1	2507.4	1038.6	3510.7	2522.1	1037.5
877.6	3611.4	2551.7	1066.9	3593.5	2561.0	1064.9	3584.8	2575.3	1063.6
898.0	3688.1	2605.5	1093.6	3669.2	2614.4	1091.4	3658.9	2628.2	1089.8
918.4	3765.4	2659.4	1120.4	3745.2	2667.7	1117.9	3733.1	2680.7	1116.0
938.8	3843.1	2713.2	1147.4	3821.6	2720.9	1144.5	3807.5	2733.0	1142.2
959.2	3921.5	2767.0	1174.5	3898.4	2774.0	1171.3	3882.1	2785.1	1168.6
979.6	4000.5	2821.0	1201.9	3975.7	2827.1	1198.3	3957.0	2837.1	1195.2
1000.0	4080.2	2875.3	1229.5	4053.6	2880.3	1225.5	4032.2	2889.2	1222.1

	T=1200			T=1500			T=1800		
P(GPa)	C11	C12	C44	C11	C12	C44	C11	C12	C44
0.0	224.3	149.4	76.6	213.7	145.2	75.0	203.3	140.9	73.4
20.4	306.9	207.0	92.7	294.7	203.3	91.9	282.7	199.5	90.9
40.8	389.6	263.9	109.2	376.2	260.5	109.2	363.0	257.0	109.0
61.2	472.4	320.4	126.1	458.0	317.2	127.1	444.1	313.8	127.6
81.6	555.2	376.6	143.6	540.2	373.6	145.4	525.7	370.3	146.8
102.0	638.0	432.8	161.5	622.7	429.9	164.2	607.9	426.7	166.4
122.4	720.7	489.0	180.0	705.3	486.3	183.4	690.5	483.2	186.5
142.9	803.3	545.3	199.0	788.0	542.8	203.1	773.5	539.9	206.9
163.3	885.9	601.8	218.5	870.8	599.6	223.1	856.7	596.9	227.6
183.7	968.2	658.6	238.4	953.6	656.8	243.6	940.0	654.4	248.6
204.1	1050.3	715.6	258.9	1036.3	714.2	264.4	1023.4	712.2	269.9
224.5	1132.2	772.8	279.7	1118.9	772.0	285.6	1106.7	770.4	291.3
244.9	1213.7	830.3	301.0	1201.3	830.0	307.1	1190.0	829.0	313.0
265.3	1295.0	888.1	322.7	1283.4	888.4	328.8	1273.1	888.0	334.9
285.7	1375.9	946.0	344.7	1365.3	947.0	350.8	1356.0	947.4	356.9
306.1	1456.5	1004.0	367.0	1447.0	1005.9	373.0	1438.6	1007.0	379.1
326.5	1536.7	1062.2	389.6	1528.2	1064.9	395.5	1520.9	1066.8	401.4
346.9	1616.6	1120.5	412.4	1609.1	1124.0	418.1	1602.9	1126.9	423.8
367.3	1696.0	1178.9	435.5	1689.7	1183.3	440.9	1684.5	1187.0	446.4
387.8	1775.1	1237.2	458.9	1769.8	1242.6	463.9	1765.7	1247.3	469.0
408.2	1853.7	1295.6	482.4	1849.6	1301.9	487.0	1846.4	1307.6	491.8
428.6	1932.0	1353.9	506.1	1928.9	1361.3	510.3	1926.8	1368.0	514.6
449.0	2010.0	1412.2	530.0	2007.9	1420.5	533.7	2006.6	1428.3	537.5
469.4	2087.5	1470.5	554.0	2086.4	1479.7	557.3	2086.1	1488.5	560.6
489.8	2164.7	1528.6	578.3	2164.5	1538.8	581.0	2165.0	1548.6	583.8
510.2	2241.6	1586.7	602.6	2242.2	1597.8	604.8	2243.5	1608.5	607.0
530.6	2318.1	1644.6	627.1	2319.5	1656.7	628.8	2321.4	1668.3	630.4
551.0	2394.3	1702.3	651.8	2396.4	1715.3	652.9	2398.9	1727.9	654.0
571.4	2470.3	1759.9	676.6	2472.9	1773.8	677.1	2476.0	1787.3	677.6
591.8	2545.9	1817.4	701.5	2549.0	1832.0	701.5	2552.5	1846.4	701.4
612.2	2621.3	1874.6	726.5	2624.8	1890.1	726.0	2628.6	1905.2	725.4
632.7	2696.4	1931.7	751.7	2700.2	1947.8	750.6	2704.2	1963.8	749.5
653.1	2771.2	1988.5	777.0	2775.2	2005.3	775.4	2779.3	2022.0	773.7
673.5	2845.8	2045.1	802.4	2849.9	2062.5	800.3	2854.0	2079.8	798.1
693.9	2920.2	2101.4	827.8	2924.2	2119.3	825.3	2928.2	2137.2	822.7
714.3	2994.4	2157.4	853.4	2998.1	2175.8	850.5	3001.9	2194.1	847.5
734.7	3068.3	2213.1	879.1	3071.7	2231.8	875.8	3075.1	2250.6	872.4
755.1	3142.0	2268.5	904.8	3145.0	2287.4	901.2	3147.9	2306.5	897.5
775.5	3215.6	2323.5	930.7	3217.9	2342.6	926.7	3220.2	2361.9	922.8
795.9	3288.9	2378.0	956.5	3290.5	2397.2	952.4	3292.0	2416.6	948.3
816.3	3362.0	2432.2	982.5	3362.7	2451.3	978.1	3363.3	2470.7	973.9
836.7	3434.9	2485.9	1008.4	3434.5	2504.9	1004.0	3434.2	2524.2	999.8
857.1	3507.7	2539.1	1034.4	3506.1	2557.8	1030.1	3504.6	2576.9	1025.9
877.6	3580.3	2591.9	1060.5	3577.3	2610.2	1056.2	3574.6	2628.9	1052.2
898.0	3652.8	2644.2	1086.6	3648.3	2662.0	1082.5	3644.1	2680.2	1078.7
918.4	3725.2	2696.1	1112.8	3718.9	2713.2	1108.9	3713.1	2730.8	1105.4
938.8	3797.5	2747.6	1139.1	3789.3	2763.9	1135.4	3781.8	2780.7	1132.4
959.2	3869.8	2798.8	1165.5	3859.6	2814.1	1162.2	3850.2	2830.1	1159.7
979.6	3942.2	2849.7	1192.1	3929.7	2864.0	1189.3	3918.3	2879.0	1187.2
1000.0	4014.7	2900.6	1219.0	3999.8	2913.7	1216.6	3986.1	2927.6	1215.1

	T=2100			T=2400			T=2700		
P(GPa)	C11	C12	C44	C11	C12	C44	C11	C12	C44
0.0	193.2	136.4	71.5	183.6	131.6	69.4	174.3	126.7	67.2
20.4	271.4	195.4	89.7	260.9	191.1	88.6	250.8	186.5	87.5
40.8	350.7	253.2	108.6	339.4	249.2	108.5	328.5	244.9	108.3
61.2	431.0	310.2	128.1	419.0	306.4	128.8	407.5	302.3	129.5
81.6	512.2	366.8	148.1	499.6	363.2	149.6	487.6	359.3	151.0
102.0	594.1	423.3	168.5	581.1	419.8	170.7	568.6	416.1	172.7
122.4	676.6	479.9	189.3	663.2	476.6	192.0	650.4	473.0	194.6
142.9	759.6	536.8	210.3	746.0	533.6	213.5	732.9	530.2	216.5
163.3	842.9	594.0	231.6	829.3	591.1	235.2	816.0	587.9	238.5
183.7	926.6	651.7	253.1	913.0	649.0	257.0	899.6	646.0	260.6
204.1	1010.4	709.9	274.7	996.9	707.5	278.8	983.4	704.8	282.6
224.5	1094.3	768.5	296.5	1081.0	766.5	300.7	1067.5	764.0	304.6
244.9	1178.3	827.7	318.3	1165.2	826.0	322.6	1151.8	823.9	326.5
265.3	1262.1	887.2	340.3	1249.4	886.1	344.6	1236.0	884.3	348.4
285.7	1345.8	947.2	362.3	1333.6	946.6	366.5	1320.2	945.2	370.3
306.1	1429.2	1007.5	384.4	1417.5	1007.5	388.5	1404.3	1006.5	392.1
326.5	1512.4	1068.1	406.6	1501.3	1068.7	410.5	1488.2	1068.2	413.9
346.9	1595.3	1129.0	428.8	1584.7	1130.2	432.5	1571.8	1130.1	435.6
367.3	1677.8	1190.0	451.1	1667.8	1192.0	454.5	1655.1	1192.3	457.3
387.8	1759.9	1251.2	473.4	1750.5	1253.9	476.5	1738.0	1254.7	479.1
408.2	1841.5	1312.4	495.8	1832.8	1315.8	498.5	1820.4	1317.2	500.8
428.6	1922.7	1373.6	518.2	1914.6	1377.8	520.7	1902.4	1379.8	522.6
449.0	2003.4	1434.9	540.7	1996.0	1439.8	542.8	1983.9	1442.3	544.5
469.4	2083.6	1496.0	563.3	2076.8	1501.7	565.1	2064.9	1504.7	566.4
489.8	2163.3	1557.0	586.0	2157.1	1563.5	587.4	2145.3	1567.0	588.4
510.2	2242.4	1617.9	608.8	2236.8	1625.2	609.9	2225.1	1629.2	610.6
530.6	2321.1	1678.6	631.8	2315.9	1686.6	632.4	2304.3	1691.2	632.8
551.0	2399.1	1739.1	654.8	2394.4	1747.8	655.1	2382.9	1752.8	655.2
571.4	2476.6	1799.3	678.0	2472.3	1808.7	678.0	2460.9	1814.2	677.8
591.8	2553.6	1859.2	701.3	2549.7	1869.3	701.0	2538.3	1875.3	700.5
612.2	2630.0	1918.8	724.8	2626.4	1929.5	724.2	2615.0	1936.0	723.5
632.7	2705.8	1978.1	748.4	2702.4	1989.4	747.6	2691.0	1996.3	746.7
653.1	2781.1	2036.9	772.3	2777.9	2048.8	771.1	2766.3	2056.1	770.1
673.5	2855.8	2095.4	796.3	2852.6	2107.7	795.0	2841.0	2115.4	793.8
693.9	2929.9	2153.3	820.5	2926.8	2166.1	819.0	2915.0	2174.2	817.8
714.3	3003.5	2210.7	845.0	3000.2	2224.0	843.3	2988.2	2232.3	842.0
734.7	3076.5	2267.6	869.6	3073.0	2281.2	867.9	3060.8	2289.9	866.5
755.1	3148.8	2323.9	894.5	3145.1	2337.8	892.7	3132.6	2346.7	891.4
775.5	3220.6	2379.5	919.7	3216.5	2393.6	917.8	3203.7	2402.7	916.6
795.9	3291.8	2434.4	945.0	3287.2	2448.7	943.2	3274.1	2458.0	942.2
816.3	3362.4	2488.6	970.7	3357.3	2503.0	969.0	3343.7	2512.4	968.1
836.7	3432.4	2542.0	996.6	3426.6	2556.4	995.0	3412.5	2565.9	994.4
857.1	3501.8	2594.5	1022.8	3495.2	2608.9	1021.4	3480.6	2618.5	1021.0
877.6	3570.6	2646.3	1049.3	3563.1	2660.5	1048.1	3548.0	2670.1	1048.1
898.0	3638.8	2697.2	1076.1	3630.3	2711.2	1075.2	3614.6	2720.7	1075.6
918.4	3706.5	2747.3	1103.1	3696.8	2760.9	1102.7	3680.5	2770.3	1103.5
938.8	3773.6	2796.6	1130.6	3762.6	2809.9	1130.5	3745.6	2819.1	1131.9
959.2	3840.3	2845.2	1158.3	3827.9	2858.0	1158.7	3810.1	2866.9	1160.7
979.6	3906.5	2893.3	1186.4	3892.6	2905.4	1187.4	3874.0	2914.1	1190.0
1000.0	3972.3	2940.9	1214.9	3956.8	2952.3	1216.5	3937.3	2960.6	1219.8

	T=3000			T=3500			T=4000		
P(GPa)	C11	C12	C44	C11	C12	C44	C11	C12	C44
0.0	165.4	121.9	65.1	152.8	115.5	63.9	140.6	109.7	62.5
20.4	241.0	182.0	86.5	226.0	175.2	86.1	211.7	168.8	85.4
40.8	318.1	240.6	108.2	301.5	233.6	108.8	285.5	226.7	108.8
61.2	396.5	298.2	130.2	378.7	291.2	131.6	361.6	284.1	132.4
81.6	476.2	355.4	152.4	457.5	348.4	154.6	439.5	341.1	156.1
102.0	556.8	412.3	174.7	537.5	405.5	177.7	518.9	398.2	179.8
122.4	638.3	469.4	197.0	618.5	462.7	200.7	599.4	455.5	203.4
142.9	720.5	526.7	219.4	700.3	520.2	223.5	680.8	513.1	226.7
163.3	803.3	584.5	241.7	782.7	578.2	246.3	762.7	571.1	249.9
183.7	886.6	642.8	263.9	865.5	636.7	268.8	845.1	629.7	272.8
204.1	970.2	701.6	286.1	948.6	695.7	291.1	927.7	688.8	295.4
224.5	1054.0	761.1	308.1	1031.8	755.3	313.3	1010.3	748.5	317.6
244.9	1137.9	821.1	330.1	1115.0	815.4	335.2	1092.8	808.8	339.6
265.3	1221.8	881.6	351.9	1198.2	876.1	357.0	1175.2	869.5	361.3
285.7	1305.7	942.7	373.6	1281.1	937.3	378.5	1257.3	930.8	382.8
306.1	1389.4	1004.1	395.3	1363.8	998.8	399.9	1339.1	992.4	404.0
326.5	1472.8	1066.0	416.8	1446.2	1060.8	421.2	1420.5	1054.4	425.0
346.9	1556.0	1128.2	438.3	1528.3	1123.0	442.3	1501.4	1116.7	445.9
367.3	1638.9	1190.6	459.8	1609.9	1185.5	463.4	1581.8	1179.2	466.6
387.8	1721.3	1253.2	481.3	1691.1	1248.1	484.4	1661.8	1241.8	487.2
408.2	1803.3	1315.9	502.7	1771.7	1310.9	505.5	1741.1	1304.6	507.8
428.6	1884.9	1378.6	524.2	1851.9	1373.7	526.5	1819.9	1367.4	528.4
449.0	1965.9	1441.4	545.8	1931.5	1436.5	547.5	1898.2	1430.2	549.0
469.4	2046.4	1504.1	567.4	2010.6	1499.2	568.7	1975.8	1492.9	569.7
489.8	2126.3	1566.6	589.1	2089.0	1561.8	589.9	2052.9	1555.5	590.5
510.2	2205.7	1629.0	610.9	2166.9	1624.2	611.3	2129.4	1618.0	611.4
530.6	2284.4	1691.2	632.9	2244.3	1686.4	632.9	2205.3	1680.2	632.6
551.0	2362.6	1753.1	655.1	2321.0	1748.4	654.6	2280.6	1742.2	653.9
571.4	2440.1	1814.8	677.4	2397.1	1810.1	676.6	2355.3	1803.8	675.6
591.8	2517.0	1876.1	700.0	2472.6	1871.4	698.9	2429.4	1865.2	697.5
612.2	2593.2	1937.0	722.8	2547.5	1932.4	721.4	2503.0	1926.2	719.7
632.7	2668.8	1997.5	745.8	2621.8	1992.9	744.2	2576.0	1986.7	742.4
653.1	2743.7	2057.5	769.2	2695.5	2053.0	767.4	2648.4	2046.9	765.4
673.5	2817.9	2117.1	792.8	2768.5	2112.6	791.0	2720.3	2106.5	788.8
693.9	2891.5	2176.0	816.7	2841.0	2171.7	814.9	2791.7	2165.6	812.7
714.3	2964.4	2234.4	841.0	2912.9	2230.2	839.2	2862.5	2224.2	837.1
734.7	3036.6	2292.1	865.6	2984.3	2288.0	864.0	2932.9	2282.1	862.0
755.1	3108.1	2349.1	890.6	3055.0	2345.2	889.2	3002.8	2339.4	887.4
775.5	3178.9	2405.4	916.0	3125.1	2401.6	915.0	3072.2	2396.0	913.4
795.9	3249.0	2460.8	941.8	3194.7	2457.3	941.2	3141.2	2451.8	940.1
816.3	3318.4	2515.4	968.0	3263.8	2512.1	967.9	3209.7	2506.9	967.3
836.7	3387.1	2569.0	994.6	3332.3	2566.0	995.2	3277.9	2561.1	995.3
857.1	3455.0	2621.7	1021.7	3400.2	2619.1	1023.1	3345.7	2614.4	1023.9
877.6	3522.3	2673.5	1049.3	3467.6	2671.2	1051.5	3413.1	2666.9	1053.2
898.0	3588.8	2724.2	1077.3	3534.5	2722.4	1080.6	3480.2	2718.4	1083.2
918.4	3654.7	2774.0	1105.8	3600.9	2772.6	1110.3	3546.9	2769.0	1114.0
938.8	3719.9	2822.8	1134.9	3666.8	2821.8	1140.6	3613.3	2818.7	1145.5
959.2	3784.4	2870.8	1164.4	3732.3	2870.2	1171.5	3679.4	2867.6	1177.9
979.6	3848.3	2917.9	1194.5	3797.2	2917.8	1203.1	3745.2	2915.6	1210.9
1000.0	3911.7	2964.5	1225.1	3861.7	2964.8	1235.3	3810.6	2963.0	1244.8