INDIAN INSTITUTE OF TECHNOLOGY INDORE

*Department of Metallurgy Engineering and Materials Science (MEMS)*



**MM 309**

**LAMMPS Output**

**“Application of Molecular dynamics (MD) in Materials Science and Engineering”.**

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**Submitted By-**

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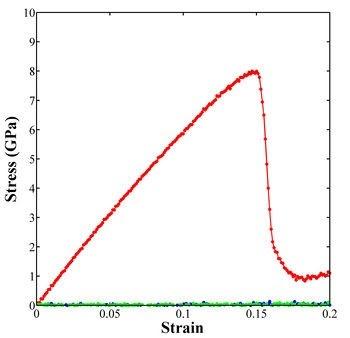
* **LAMMPS Example-1 OUTPUT**

1. Logfile data

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| LAMMPS (29 Sep 2021)  OMP\_NUM\_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)  using 1 OpenMP thread(s) per MPI task  # Input file for uniaxial tensile loading of single crystal aluminum  # ------------------------ INITIALIZATION ----------------------------  units metal  dimension 3  boundary p p p  atom\_style atomic  variable latparam equal 4.05  # ----------------------- ATOM DEFINITION ----------------------------  lattice fcc ${latparam}  lattice fcc 4.05  Lattice spacing in x,y,z = 4.0500000 4.0500000 4.0500000  region whole block 0 10 0 10 0 10  create\_box 1 whole  Created orthogonal box = (0.0000000 0.0000000 0.0000000) to (40.500000 40.500000 40.500000)  1 by 1 by 1 MPI processor grid  lattice fcc ${latparam} orient x 1 0 0 orient y 0 1 0 orient z 0 0 1  lattice fcc 4.05 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1  Lattice spacing in x,y,z = 4.0500000 4.0500000 4.0500000  create\_atoms 1 region whole  Created 4000 atoms  using lattice units in orthogonal box = (0.0000000 0.0000000 0.0000000) to (40.500000 40.500000 40.500000)  create\_atoms CPU = 0.003 seconds  # ------------------------ FORCE FIELDS ------------------------------  pair\_style eam/alloy  pair\_coeff \* \* Al99.eam.alloy Al  # ------------------------- SETTINGS ---------------------------------  compute csym all centro/atom fcc  compute peratom all pe/atom  ######################################  # EQUILIBRATION  reset\_timestep 0  timestep 0.001  velocity all create 300 12345 mom yes rot no  fix 1 all npt temp 300 300 1 iso 0 0 1 drag 1  # Set thermo output  thermo 1000  thermo\_style custom step lx ly lz press pxx pyy pzz pe temp  # Run for at least 10 picosecond (assuming 1 fs timestep)  run 20000  Neighbor list info ...  update every 1 steps, delay 10 steps, check yes  max neighbors/atom: 2000, page size: 100000  master list distance cutoff = 8.28721  ghost atom cutoff = 8.28721  binsize = 4.143605, bins = 10 10 10  2 neighbor lists, perpetual/occasional/extra = 1 1 0  (1) pair eam/alloy, perpetual  attributes: half, newton on  pair build: half/bin/atomonly/newton  stencil: half/bin/3d  bin: standard  (2) compute centro/atom, occasional  attributes: full, newton on  pair build: full/bin/atomonly  stencil: full/bin/3d  bin: standard  Per MPI rank memory allocation (min/avg/max) = 5.218 | 5.218 | 5.218 Mbytes  Step Lx Ly Lz Press Pxx Pyy Pzz PotEng Temp  0 40.5 40.5 40.5 2496.1233 2446.9902 2534.6541 2506.7256 -13440 300  1000 40.557742 40.557742 40.557742 780.10773 768.50566 776.04263 795.77489 -13363.126 169.17189  2000 40.573581 40.573581 40.573581 85.256296 2.5136289 170.1902 83.065057 -13356.006 178.00901  3000 40.580468 40.580468 40.580468 225.24624 185.42636 364.5654 125.74696 -13346.557 182.73335  4000 40.588153 40.588153 40.588153 36.447911 18.973498 31.021312 59.348922 -13340.448 193.9013  5000 40.591847 40.591847 40.591847 182.0974 68.023328 389.00854 89.260333 -13335.805 207.68103  6000 40.595764 40.595764 40.595764 321.87463 190.03025 561.47818 214.11546 -13329.141 217.01995  7000 40.603317 40.603317 40.603317 362.92787 368.19237 401.37129 319.21994 -13320.261 221.3218  8000 40.611092 40.611092 40.611092 101.44517 163.35387 -22.286553 163.26819 -13316.435 234.4251  9000 40.618228 40.618228 40.618228 48.335417 -28.184491 19.629696 153.56105 -13314.162 249.30546  10000 40.625527 40.625527 40.625527 23.640617 47.427825 -67.271183 90.765209 -13307.557 254.39739  11000 40.629423 40.629423 40.629423 14.930363 86.558582 -86.67342 44.905927 -13303.421 262.70399  12000 40.632725 40.632725 40.632725 -61.882766 19.125643 -151.76692 -53.007018 -13301.159 272.96087  13000 40.636203 40.636203 40.636203 36.702053 84.733127 142.408 -117.03497 -13298.549 280.79394  14000 40.641711 40.641711 40.641711 -181.21685 -153.98286 -220.08985 -169.57783 -13295.754 286.5089  15000 40.645191 40.645191 40.645191 -129.63386 -64.948063 -286.84124 -37.112278 -13290.696 286.09792  16000 40.645446 40.645446 40.645446 -39.533108 -10.232785 -21.609937 -86.756601 -13289.355 291.21878  17000 40.648885 40.648885 40.648885 -148.25118 -220.97994 -282.82076 59.047162 -13288.768 296.23678  18000 40.646623 40.646623 40.646623 67.624312 74.684518 59.767756 68.420662 -13287.047 297.52126  19000 40.645806 40.645806 40.645806 131.77506 4.118904 349.42952 41.776761 -13285.602 297.93361  20000 40.65015 40.65015 40.65015 -120.83606 -65.442048 -112.76929 -184.29685 -13286.614 301.79878  Loop time of 332.919 on 1 procs for 20000 steps with 4000 atoms  Performance: 5.190 ns/day, 4.624 hours/ns, 60.075 timesteps/s  94.6% CPU use with 1 MPI tasks x 1 OpenMP threads  MPI task timing breakdown:  Section | min time | avg time | max time |%varavg| %total  ---------------------------------------------------------------  Pair | 324.68 | 324.68 | 324.68 | 0.0 | 97.52  Neigh | 0 | 0 | 0 | 0.0 | 0.00  Comm | 1.3746 | 1.3746 | 1.3746 | 0.0 | 0.41  Output | 0.0031397 | 0.0031397 | 0.0031397 | 0.0 | 0.00  Modify | 5.8908 | 5.8908 | 5.8908 | 0.0 | 1.77  Other | | 0.9715 | | | 0.29  Nlocal: 4000.00 ave 4000 max 4000 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Nghost: 8195.00 ave 8195 max 8195 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Neighs: 280000.0 ave 280000 max 280000 min  Histogram: 1 0 0 0 0 0 0 0 0 0  FullNghs: 0.00000 ave 0 max 0 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Total # of neighbors = 280000  Ave neighs/atom = 70.000000  Neighbor list builds = 0  Dangerous builds = 0  unfix 1  # Store final cell length for strain calculations  variable tmp equal "lx"  variable L0 equal ${tmp}  variable L0 equal 40.650149791353  print "Initial Length, L0: ${L0}"  Initial Length, L0: 40.650149791353  ######################################  # DEFORMATION  reset\_timestep 0  fix 1 all npt temp 300 300 1 y 0 0 1 z 0 0 1 drag 1  variable srate equal 1.0e10  variable srate1 equal "v\_srate / 1.0e12"  fix 2 all deform 1 x erate ${srate1} units box remap x  fix 2 all deform 1 x erate 0.01 units box remap x  # Output strain and stress info to file  # for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]  # p2, p3, p4 are in GPa  variable strain equal "(lx - v\_L0)/v\_L0"  variable p1 equal "v\_strain"  variable p2 equal "-pxx/10000"  variable p3 equal "-pyy/10000"  variable p4 equal "-pzz/10000"  fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file Al\_SC\_100.def1.txt screen no  # Use cfg for AtomEye  dump 1 all cfg 250 dump.tensile\_\*.cfg mass type xs ys zs c\_csym c\_peratom fx fy fz  dump\_modify 1 element Al  # Display thermo  thermo 1000  thermo\_style custom step v\_strain temp v\_p2 v\_p3 v\_p4 ke pe press  run 20000  Per MPI rank memory allocation (min/avg/max) = 8.934 | 8.934 | 8.934 Mbytes  Step v\_strain Temp v\_p2 v\_p3 v\_p4 KinEng PotEng Press  0 3.4958923e-16 301.79878 0.0065442048 0.011276929 0.018429685 156.00321 -13286.614 -120.83606  1000 0.01 299.89338 0.63310591 0.026431004 -0.025006804 155.01828 -13283.121 -2115.1004  2000 0.02 299.98278 1.2734386 0.026640905 -0.031038545 155.06449 -13277.768 -4230.1366  3000 0.03 299.03654 1.8866341 -0.0039516101 -0.027300257 154.57537 -13269.139 -6184.6074  4000 0.04 296.78316 2.5173859 0.001190575 0.006627888 153.41058 -13257.188 -8417.3479  5000 0.05 297.45562 3.1275098 0.00081509981 0.0044511143 153.75818 -13244.232 -10442.587  6000 0.06 296.51822 3.7297819 0.0056687276 0.087908414 153.27363 -13228.034 -12744.53  7000 0.07 299.91171 4.2690469 -0.0050984108 -0.027100188 155.02776 -13211.678 -14122.828  8000 0.08 295.95815 4.8006899 -0.075117832 -0.051869757 152.98412 -13189.161 -15579.008  9000 0.09 300.87708 5.3719796 -0.012591905 -0.011921464 155.52677 -13169.052 -17824.888  10000 0.1 295.4211 5.9324088 -0.026778173 0.038661531 152.70651 -13141.376 -19814.307  11000 0.11 303.12092 6.4923293 0.038459848 -0.04497285 156.68663 -13118.186 -21619.388  12000 0.12 296.63854 6.9942211 0.0015475437 0.11986661 153.33582 -13085.545 -23718.784  13000 0.13 295.55374 7.4533589 0.056040516 0.02077978 152.77508 -13053.558 -25100.597  14000 0.14 295.07115 7.8092372 -0.028582597 -0.020564904 152.52562 -13020.052 -25866.966  15000 0.15 292.31178 7.9115913 0.029197225 0.069420705 151.09927 -12983.712 -26700.697  16000 0.16 392.35968 2.4155358 0.075370042 0.0062644364 202.81516 -13020.131 -8323.9009  17000 0.17 400.90581 1.8827775 0.011578053 0.022483542 207.23275 -13036.882 -6389.4638  18000 0.18 414.22996 0.97799795 -0.064019183 0.0029853052 214.12016 -13061.813 -3056.5469  19000 0.19 412.23366 0.88392893 -0.0033189151 -0.085427937 213.08824 -13081.998 -2650.6069  20000 0.2 408.31271 1.0402719 0.039376419 -0.0085543025 211.06146 -13101.996 -3570.3134  Loop time of 324.393 on 1 procs for 20000 steps with 4000 atoms  Performance: 5.327 ns/day, 4.505 hours/ns, 61.654 timesteps/s  95.1% CPU use with 1 MPI tasks x 1 OpenMP threads  MPI task timing breakdown:  Section | min time | avg time | max time |%varavg| %total  ---------------------------------------------------------------  Pair | 308.25 | 308.25 | 308.25 | 0.0 | 95.02  Neigh | 1.0177 | 1.0177 | 1.0177 | 0.0 | 0.31  Comm | 1.1158 | 1.1158 | 1.1158 | 0.0 | 0.34  Output | 6.2395 | 6.2395 | 6.2395 | 0.0 | 1.92  Modify | 7.0861 | 7.0861 | 7.0861 | 0.0 | 2.18  Other | | 0.6842 | | | 0.21  Nlocal: 4000.00 ave 4000 max 4000 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Nghost: 7144.00 ave 7144 max 7144 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Neighs: 276477.0 ave 276477 max 276477 min  Histogram: 1 0 0 0 0 0 0 0 0 0  FullNghs: 552303.0 ave 552303 max 552303 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Total # of neighbors = 552303  Ave neighs/atom = 138.07575  Neighbor list builds = 85  Dangerous builds = 0  ######################################  # SIMULATION DONE  print "All done"  All done  Total wall time: 0:10:57 |

1. **Stress-Strain Plot**

“File Al\_SC\_100.def1.txt “ is created after simulation. Using the **MATLAB** software,The stress-strain curve is plotted.



* **MATLAB Code**

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| **%% Analyze def1.txt files**  **% Plot the various responses**  **d = dir('\*.def1.txt');**  **for i = 1:length(d)**  **% Get data**  **fname = d(i).name;**  **A = importdata(fname);**  **strain = A.data(:,1);**  **stress = A.data(:,2:4);**  **% Generate plot**  **plot(strain,stress(:,1),'-or','LineWidth',2,'MarkerEdgeColor','r',...**  **'MarkerFaceColor','r','MarkerSize',5),hold on**  **plot(strain,stress(:,2),'-ob','LineWidth',2,'MarkerEdgeColor','b',...**  **'MarkerFaceColor','b','MarkerSize',5),hold on**  **plot(strain,stress(:,3),'-og','LineWidth',2,'MarkerEdgeColor','g',...**  **'MarkerFaceColor','g','MarkerSize',5),hold on**  **axis square**  **ylim([0 10])**  **set(gca,'LineWidth',2,'FontSize',24,'FontWeight','normal','FontName','Times')**  **set(get(gca,'XLabel'),'String','Strain','FontSize',32,'FontWeight','bold','FontName','Times')**  **set(get(gca,'YLabel'),'String','Stress (GPa)','FontSize',32,'FontWeight','bold','FontName','Times')**  **set(gcf,'Position',[1 1 round(1000) round(1000)])**  **% Export figure to tif file**  **exportfig(gcf,strrep(fname,'.def1.txt','.tif'),'Format','tiff',...**  **'Color','rgb','Resolution',300)**  **close(1)**  **end** |

1. **OVITO output**

Video link:--

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| <https://drive.google.com/file/d/1ny-5x_N-YUI28IaEyNp5eLXBggS1yi67/view?usp=sharing> |

* **LAMMPS Example-2 OUTPUT**

1. logfile data

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| LAMMPS (29 Sep 2021)  OMP\_NUM\_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)  using 1 OpenMP thread(s) per MPI task  # LAMMPS Input File for Grain Boundaries  # This file will generate a single Sigma5(310) STGB  # ---------- Initialize Simulation ---------------------  clear  OMP\_NUM\_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)  using 1 OpenMP thread(s) per MPI task  units metal  dimension 3  boundary p p p  atom\_style atomic  # ---------- Create Atomistic Structure ---------------------  lattice fcc 4.05  Lattice spacing in x,y,z = 4.0500000 4.0500000 4.0500000  region whole block 0.000000 12.807225 -64.0361225 64.0361225 0.000000 4.050000 units box  create\_box 2 whole  Created orthogonal box = (0.0000000 -64.036123 0.0000000) to (12.807225 64.036123 4.0500000)  1 by 1 by 1 MPI processor grid  region upper block INF INF 0.000000 64.0361225 INF INF units box  lattice fcc 4.05 orient x 0 3 1 orient y 0 -1 3 orient z 1 0 0  Lattice spacing in x,y,z = 5.1228898 5.1228898 4.0500000  create\_atoms 1 region upper  Created 200 atoms  using lattice units in orthogonal box = (0.0000000 -64.036123 0.0000000) to (12.807225 64.036123 4.0500000)  create\_atoms CPU = 0.001 seconds  region lower block INF INF -64.0361225 0.000000 INF INF units box  lattice fcc 4.05 orient x 0 3 -1 orient y 0 1 3 orient z 1 0 0  Lattice spacing in x,y,z = 5.1228898 5.1228898 4.0500000  create\_atoms 2 region lower  Created 200 atoms  using lattice units in orthogonal box = (0.0000000 -64.036123 0.0000000) to (12.807225 64.036123 4.0500000)  create\_atoms CPU = 0.000 seconds  group upper type 1  200 atoms in group upper  group lower type 2  200 atoms in group lower  # ---------- Define Interatomic Potential ---------------------  pair\_style eam/alloy  pair\_coeff \* \* Al99.eam.alloy Al Al  neighbor 2.0 bin  neigh\_modify delay 10 check yes  # ---------- Displace atoms and delete overlapping atoms ---------------------  displace\_atoms upper move 0 0 0 units lattice  Displacing atoms ...  delete\_atoms overlap 0.35 lower upper  System init for delete\_atoms ...  Neighbor list info ...  update every 1 steps, delay 10 steps, check yes  max neighbors/atom: 2000, page size: 100000  master list distance cutoff = 8.28721  ghost atom cutoff = 8.28721  binsize = 4.143605, bins = 4 31 1  2 neighbor lists, perpetual/occasional/extra = 1 1 0  (1) command delete\_atoms, occasional  attributes: full, newton on  pair build: full/bin/atomonly  stencil: full/bin/3d  bin: standard  (2) pair eam/alloy, perpetual  attributes: half, newton on  pair build: half/bin/atomonly/newton  stencil: half/bin/3d  bin: standard  Deleted 2 atoms, new total = 398  # ---------- Define Settings ---------------------  compute csym all centro/atom fcc  compute eng all pe/atom  compute eatoms all reduce sum c\_eng  # ---------- Run Minimization ---------------------  reset\_timestep 0  thermo 10  thermo\_style custom step pe lx ly lz press pxx pyy pzz c\_eatoms  dump 1 all cfg 25 dump.sig5\_minimization\_\*.cfg mass type xs ys zs c\_csym c\_eng fx fy fz  dump\_modify 1 element Al Al  min\_style cg  minimize 1e-15 1e-15 5000 5000  WARNING: Using 'neigh\_modify every 1 delay 0 check yes' setting during minimization (src/min.cpp:188)  Neighbor list info ...  update every 1 steps, delay 0 steps, check yes  max neighbors/atom: 2000, page size: 100000  master list distance cutoff = 8.28721  ghost atom cutoff = 8.28721  binsize = 4.143605, bins = 4 31 1  2 neighbor lists, perpetual/occasional/extra = 1 1 0  (1) pair eam/alloy, perpetual  attributes: half, newton on  pair build: half/bin/atomonly/newton  stencil: half/bin/3d  bin: standard  (2) compute centro/atom, occasional  attributes: full, newton on  pair build: full/bin/atomonly  stencil: full/bin/3d  bin: standard  Per MPI rank memory allocation (min/avg/max) = 6.915 | 6.915 | 6.915 Mbytes  Step PotEng Lx Ly Lz Press Pxx Pyy Pzz c\_eatoms  0 -1318.9843 12.807225 128.07225 4.05 875.32429 -2675.7752 7333.2608 -2031.5128 -1318.9843  10 -1329.8293 12.807225 128.07225 4.05 4863.0678 2399.3262 9226.618 2963.2592 -1329.8293  20 -1330.1813 12.807225 128.07225 4.05 5739.7373 3277.6653 10380.205 3561.3418 -1330.1813  30 -1330.212 12.807225 128.07225 4.05 5799.4078 3324.6136 10511.649 3561.9611 -1330.212  40 -1330.2137 12.807225 128.07225 4.05 5823.0131 3345.3792 10560.649 3563.0112 -1330.2137  50 -1330.2144 12.807225 128.07225 4.05 5832.2375 3357.8939 10569.301 3569.5176 -1330.2144  60 -1330.2146 12.807225 128.07225 4.05 5829.3139 3356.4392 10559.179 3572.3232 -1330.2146  70 -1330.2147 12.807225 128.07225 4.05 5826.5788 3359.271 10546.817 3573.6486 -1330.2147  80 -1330.2148 12.807225 128.07225 4.05 5827.0603 3369.2954 10538.855 3573.031 -1330.2148  90 -1330.2149 12.807225 128.07225 4.05 5827.8483 3370.9088 10540.535 3572.1008 -1330.2149  100 -1330.2149 12.807225 128.07225 4.05 5827.4309 3370.2637 10540.434 3571.5951 -1330.2149  110 -1330.2149 12.807225 128.07225 4.05 5827.2641 3370.103 10540.1 3571.5894 -1330.2149  120 -1330.2149 12.807225 128.07225 4.05 5827.1959 3370.2252 10539.733 3571.6293 -1330.2149  130 -1330.2149 12.807225 128.07225 4.05 5827.2147 3370.2646 10539.782 3571.5977 -1330.2149  140 -1330.2149 12.807225 128.07225 4.05 5827.2184 3370.2755 10539.789 3571.5903 -1330.2149  150 -1330.2149 12.807225 128.07225 4.05 5827.2224 3370.2832 10539.793 3571.5908 -1330.2149  160 -1330.2184 12.807225 128.07225 4.05 5890.1006 3593.9061 10554.021 3522.3744 -1330.2184  170 -1331.0778 12.807225 128.07225 4.05 3363.4114 1976.0181 6867.2229 1246.9931 -1331.0778  180 -1332.2028 12.807225 128.07225 4.05 887.83423 108.08119 3014.253 -458.83148 -1332.2028  190 -1332.6266 12.807225 128.07225 4.05 508.3929 -493.02789 2287.1835 -268.97693 -1332.6266  200 -1332.8494 12.807225 128.07225 4.05 584.57482 -586.13363 2641.6978 -301.83971 -1332.8494  210 -1333.1457 12.807225 128.07225 4.05 362.74086 -373.83536 1979.452 -517.3941 -1333.1457  220 -1333.2654 12.807225 128.07225 4.05 335.96609 -404.13416 1996.6089 -584.57652 -1333.2654  230 -1333.3066 12.807225 128.07225 4.05 285.92306 -449.64193 1942.4063 -634.99523 -1333.3066  240 -1333.4351 12.807225 128.07225 4.05 -158.54002 -729.53121 1235.6965 -981.78532 -1333.4351  250 -1333.5032 12.807225 128.07225 4.05 -205.75081 -678.50847 1033.4206 -972.16453 -1333.5032  260 -1333.5342 12.807225 128.07225 4.05 -39.583009 -364.88479 1252.201 -1006.0652 -1333.5342  270 -1333.5719 12.807225 128.07225 4.05 169.77134 -17.099819 1487.1073 -960.69345 -1333.5719  280 -1333.599 12.807225 128.07225 4.05 168.11579 -37.922539 1503.5999 -961.32997 -1333.599  290 -1333.6146 12.807225 128.07225 4.05 170.49145 -5.4202631 1495.7844 -978.88982 -1333.6146  300 -1333.6214 12.807225 128.07225 4.05 163.85097 -0.51008357 1471.4509 -979.38792 -1333.6214  310 -1333.6224 12.807225 128.07225 4.05 165.64539 -0.22457313 1481.3914 -984.23067 -1333.6224  320 -1333.623 12.807225 128.07225 4.05 162.51303 -2.0704805 1474.8855 -985.27592 -1333.623  330 -1333.6231 12.807225 128.07225 4.05 162.47033 -0.18879661 1473.5023 -985.90255 -1333.6231  340 -1333.6232 12.807225 128.07225 4.05 162.67746 0.069726045 1473.4338 -985.47117 -1333.6232  350 -1333.6232 12.807225 128.07225 4.05 162.88427 2.0849681 1472.3991 -985.83125 -1333.6232  360 -1333.6232 12.807225 128.07225 4.05 162.88953 2.2651336 1472.3225 -985.91908 -1333.6232  370 -1333.6232 12.807225 128.07225 4.05 162.77074 2.9347945 1471.4062 -986.02881 -1333.6232  380 -1333.6232 12.807225 128.07225 4.05 162.70892 3.3748007 1470.7803 -986.02837 -1333.6232  390 -1333.6232 12.807225 128.07225 4.05 162.71073 3.5454484 1470.6244 -986.03761 -1333.6232  400 -1333.6232 12.807225 128.07225 4.05 162.76193 3.6531303 1470.7469 -986.11421 -1333.6232  410 -1333.6232 12.807225 128.07225 4.05 162.77144 3.7039631 1470.7087 -986.09837 -1333.6232  420 -1333.6232 12.807225 128.07225 4.05 162.75774 3.6852329 1470.6866 -986.09863 -1333.6232  430 -1333.6232 12.807225 128.07225 4.05 162.7561 3.701587 1470.6666 -986.0999 -1333.6232  440 -1333.6232 12.807225 128.07225 4.05 162.75655 3.7056533 1470.6688 -986.10476 -1333.6232  450 -1333.6232 12.807225 128.07225 4.05 162.75532 3.6976367 1470.6728 -986.10443 -1333.6232  460 -1333.6232 12.807225 128.07225 4.05 162.75595 3.6991523 1470.6734 -986.10467 -1333.6232  470 -1333.6232 12.807225 128.07225 4.05 162.75646 3.7050593 1470.6699 -986.1056 -1333.6232  477 -1333.6232 12.807225 128.07225 4.05 162.75648 3.7042736 1470.6718 -986.10669 -1333.6232  Loop time of 1.88804 on 1 procs for 477 steps with 398 atoms  85.2% CPU use with 1 MPI tasks x 1 OpenMP threads  Minimization stats:  Stopping criterion = energy tolerance  Energy initial, next-to-last, final =  -1318.98429984982 -1333.62318020415 -1333.62318020415  Force two-norm initial, final = 17.588578 5.6914343e-06  Force max component initial, final = 6.2503571 1.1079118e-06  Final line search alpha, max atom move = 1.0000000 1.1079118e-06  Iterations, force evaluations = 477 930  MPI task timing breakdown:  Section | min time | avg time | max time |%varavg| %total  ---------------------------------------------------------------  Pair | 1.4733 | 1.4733 | 1.4733 | 0.0 | 78.03  Neigh | 0.00099897 | 0.00099897 | 0.00099897 | 0.0 | 0.05  Comm | 0.056697 | 0.056697 | 0.056697 | 0.0 | 3.00  Output | 0.30004 | 0.30004 | 0.30004 | 0.0 | 15.89  Modify | 0 | 0 | 0 | 0.0 | 0.00  Other | | 0.05704 | | | 3.02  Nlocal: 398.000 ave 398 max 398 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Nghost: 5281.00 ave 5281 max 5281 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Neighs: 27720.0 ave 27720 max 27720 min  Histogram: 1 0 0 0 0 0 0 0 0 0  FullNghs: 55436.0 ave 55436 max 55436 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Total # of neighbors = 55436  Ave neighs/atom = 139.28643  Neighbor list builds = 3  Dangerous builds = 0  undump 1  # ---------- Run Minimization 2---------------------  # Now allow the box to expand/contract perpendicular to the grain boundary  reset\_timestep 0  thermo 10  thermo\_style custom step pe lx ly lz press pxx pyy pzz c\_eatoms  fix 1 all box/relax y 0 vmax 0.001  min\_style cg  minimize 1e-15 1e-15 5000 5000  WARNING: Using 'neigh\_modify every 1 delay 0 check yes' setting during minimization (src/min.cpp:188)  Per MPI rank memory allocation (min/avg/max) = 5.643 | 5.643 | 5.643 Mbytes  Step PotEng Lx Ly Lz Press Pxx Pyy Pzz c\_eatoms  0 -1333.6232 12.807225 128.07225 4.05 162.75648 3.7042736 1470.6718 -986.10669 -1333.6232  10 -1333.6271 12.807225 128.23639 4.05 -843.17167 -752.01912 2.4879548 -1779.9839 -1333.6271  20 -1333.6271 12.807225 128.23694 4.05 -845.42449 -753.17452 0.50470996 -1783.6037 -1333.6271  30 -1333.6271 12.807225 128.23691 4.05 -845.75547 -753.65596 0.46149758 -1784.072 -1333.6271  40 -1333.6271 12.807225 128.23717 4.05 -846.4245 -754.23505 0.30592786 -1785.3444 -1333.6271  50 -1333.6271 12.807225 128.23732 4.05 -847.31255 -755.4133 0.433084 -1786.9574 -1333.6271  60 -1333.6271 12.807225 128.23717 4.05 -846.43603 -754.47227 0.38986353 -1785.2257 -1333.6271  70 -1333.6271 12.807225 128.23722 4.05 -846.82106 -754.95806 0.36230166 -1785.8674 -1333.6271  80 -1333.6271 12.807225 128.23727 4.05 -847.16656 -755.70425 0.3392705 -1786.1347 -1333.6271  90 -1333.6271 12.807225 128.23721 4.05 -846.87878 -755.31349 0.33075677 -1785.6536 -1333.6271  100 -1333.6271 12.807225 128.23722 4.05 -847.07413 -755.6895 0.31358884 -1785.8465 -1333.6271  110 -1333.6271 12.807225 128.23722 4.05 -847.09313 -756.19346 0.3157026 -1785.4016 -1333.6271  120 -1333.6271 12.807225 128.23726 4.05 -847.15194 -756.10344 0.41009355 -1785.7625 -1333.6271  130 -1333.6271 12.807225 128.23734 4.05 -847.49062 -756.14392 0.31079815 -1786.6387 -1333.6271  140 -1333.6271 12.807225 128.23733 4.05 -847.2731 -755.76001 0.4240138 -1786.4833 -1333.6271  150 -1333.6271 12.807225 128.23734 4.05 -847.32768 -755.68715 0.35080239 -1786.6467 -1333.6271  160 -1333.6271 12.807225 128.23734 4.05 -847.49834 -756.34228 0.37191668 -1786.5247 -1333.6271  170 -1333.6271 12.807225 128.23732 4.05 -847.44122 -756.74176 0.38515687 -1785.9671 -1333.6271  180 -1333.6271 12.807225 128.23734 4.05 -847.6339 -756.96389 0.31157914 -1786.2494 -1333.6271  190 -1333.6271 12.807225 128.23734 4.05 -847.8131 -757.3629 0.34183655 -1786.4183 -1333.6271  200 -1333.6271 12.807225 128.2373 4.05 -847.68052 -757.58412 0.37088417 -1785.8283 -1333.6271  210 -1333.6271 12.807225 128.23731 4.05 -847.75218 -757.61671 0.33100062 -1785.9708 -1333.6271  220 -1333.6271 12.807225 128.23737 4.05 -847.94514 -757.67105 0.39056299 -1786.5549 -1333.6271  230 -1333.6271 12.807225 128.23741 4.05 -848.05235 -758.00115 0.30565769 -1786.4616 -1333.6271  240 -1333.6271 12.807225 128.23744 4.05 -848.19022 -758.31321 0.28079337 -1786.5383 -1333.6271  250 -1333.6271 12.807225 128.23742 4.05 -848.16219 -758.28721 0.28396429 -1786.4833 -1333.6271  260 -1333.6271 12.807225 128.23742 4.05 -848.15471 -758.4768 0.23367722 -1786.221 -1333.6271  270 -1333.6271 12.807225 128.23745 4.05 -848.39173 -758.92271 0.24771911 -1786.5002 -1333.6271  280 -1333.6271 12.807225 128.23743 4.05 -848.33319 -758.90714 0.25980294 -1786.3522 -1333.6271  290 -1333.6271 12.807225 128.23741 4.05 -848.24676 -758.96019 0.24365427 -1786.0237 -1333.6271  300 -1333.6271 12.807225 128.23748 4.05 -848.60269 -759.19567 0.24299228 -1786.8554 -1333.6271  310 -1333.6271 12.807225 128.23748 4.05 -848.52593 -758.88691 0.2036751 -1786.8946 -1333.6271  320 -1333.6271 12.807225 128.23747 4.05 -848.52489 -758.92757 0.14433806 -1786.7914 -1333.6271  330 -1333.6271 12.807225 128.23753 4.05 -848.78661 -759.20053 0.14260523 -1787.3019 -1333.6271  340 -1333.6271 12.807225 128.23752 4.05 -848.62374 -759.0006 0.14594823 -1787.0166 -1333.6271  350 -1333.6271 12.807225 128.23752 4.05 -848.73081 -759.17549 0.15655087 -1787.1735 -1333.6271  360 -1333.6271 12.807225 128.23752 4.05 -848.77434 -759.16622 0.15519768 -1787.312 -1333.6271  370 -1333.6271 12.807225 128.23749 4.05 -848.52523 -758.92876 0.15073928 -1786.7977 -1333.6271  380 -1333.6271 12.807225 128.23752 4.05 -848.76248 -759.22381 0.10527089 -1787.1689 -1333.6271  390 -1333.6271 12.807225 128.23752 4.05 -848.78411 -759.29681 0.12410968 -1787.1796 -1333.6271  400 -1333.6271 12.807225 128.23749 4.05 -848.558 -759.07821 0.1471954 -1786.743 -1333.6271  410 -1333.6271 12.807225 128.23751 4.05 -848.73203 -759.20055 0.12997645 -1787.1255 -1333.6271  420 -1333.6271 12.807225 128.23753 4.05 -848.83685 -759.30871 0.14736383 -1787.3492 -1333.6271  430 -1333.6271 12.807225 128.23751 4.05 -848.65889 -759.14123 0.13402321 -1786.9695 -1333.6271  440 -1333.6271 12.807225 128.23752 4.05 -848.71415 -759.13316 0.11941479 -1787.1287 -1333.6271  450 -1333.6271 12.807225 128.23754 4.05 -848.80504 -759.16787 0.14244067 -1787.3897 -1333.6271  460 -1333.6271 12.807225 128.23751 4.05 -848.65179 -759.00837 0.12965295 -1787.0766 -1333.6271  470 -1333.6271 12.807225 128.23751 4.05 -848.61612 -758.97884 0.13414112 -1787.0037 -1333.6271  480 -1333.6271 12.807225 128.23752 4.05 -848.75612 -759.14938 0.13013127 -1787.2491 -1333.6271  490 -1333.6271 12.807225 128.2375 4.05 -848.68211 -759.16866 0.1221076 -1786.9998 -1333.6271  500 -1333.6271 12.807225 128.23749 4.05 -848.59975 -759.14129 0.1320399 -1786.79 -1333.6271  510 -1333.6271 12.807225 128.23751 4.05 -848.75033 -759.27144 0.12331834 -1787.1029 -1333.6271  520 -1333.6271 12.807225 128.2375 4.05 -848.75081 -759.25843 0.10015072 -1787.0942 -1333.6271  530 -1333.6271 12.807225 128.23748 4.05 -848.63797 -759.16659 0.086436147 -1786.8338 -1333.6271  540 -1333.6271 12.807225 128.2375 4.05 -848.71839 -759.27166 0.068793493 -1786.9523 -1333.6271  550 -1333.6271 12.807225 128.23751 4.05 -848.80249 -759.38358 0.070496223 -1787.0944 -1333.6271  560 -1333.6271 12.807225 128.2375 4.05 -848.71557 -759.31209 0.081644853 -1786.9163 -1333.6271  570 -1333.6271 12.807225 128.23749 4.05 -848.68455 -759.26725 0.086518541 -1786.8729 -1333.6271  580 -1333.6271 12.807225 128.2375 4.05 -848.78472 -759.36702 0.096497624 -1787.0836 -1333.6271  590 -1333.6271 12.807225 128.23749 4.05 -848.72812 -759.30007 0.099485885 -1786.9838 -1333.6271  600 -1333.6271 12.807225 128.23748 4.05 -848.6151 -759.10125 0.11276428 -1786.8568 -1333.6271  610 -1333.6271 12.807225 128.2375 4.05 -848.68959 -759.08015 0.11900782 -1787.1076 -1333.6271  620 -1333.6271 12.807225 128.23749 4.05 -848.62054 -758.92185 0.14120283 -1787.081 -1333.6271  630 -1333.6271 12.807225 128.23747 4.05 -848.45165 -758.61771 0.13313349 -1786.8704 -1333.6271  640 -1333.6271 12.807225 128.23748 4.05 -848.50872 -758.55293 0.12937935 -1787.1026 -1333.6271  650 -1333.6271 12.807225 128.23748 4.05 -848.50023 -758.50043 0.10662403 -1787.1069 -1333.6271  660 -1333.6271 12.807225 128.23747 4.05 -848.38178 -758.31644 0.088822148 -1786.9177 -1333.6271  670 -1333.6271 12.807225 128.23747 4.05 -848.42614 -758.32819 0.089834003 -1787.0401 -1333.6271  680 -1333.6271 12.807225 128.23747 4.05 -848.40837 -758.33493 0.098100723 -1786.9883 -1333.6271  690 -1333.6271 12.807225 128.23744 4.05 -848.23826 -758.14397 0.11150997 -1786.6823 -1333.6271  700 -1333.6271 12.807225 128.23743 4.05 -848.25786 -758.11892 0.1053529 -1786.76 -1333.6271  710 -1333.6271 12.807225 128.23744 4.05 -848.28494 -758.16576 0.11337144 -1786.8024 -1333.6271  720 -1333.6271 12.807225 128.23742 4.05 -848.184 -758.05662 0.10621874 -1786.6016 -1333.6271  730 -1333.6271 12.807225 128.23741 4.05 -848.16483 -758.02187 0.12631132 -1786.5989 -1333.6271  740 -1333.6271 12.807225 128.23742 4.05 -848.20346 -758.09635 0.12103079 -1786.6351 -1333.6271  750 -1333.6271 12.807225 128.23741 4.05 -848.14141 -758.01752 0.10920231 -1786.5159 -1333.6271  760 -1333.6271 12.807225 128.23741 4.05 -848.14428 -757.96274 0.10240074 -1786.5725 -1333.6271  770 -1333.6271 12.807225 128.23741 4.05 -848.17081 -757.9829 0.089972207 -1786.6195 -1333.6271  780 -1333.6271 12.807225 128.23741 4.05 -848.11674 -757.91668 0.08797264 -1786.5215 -1333.6271  790 -1333.6271 12.807225 128.23741 4.05 -848.09941 -757.84892 0.084031708 -1786.5333 -1333.6271  800 -1333.6271 12.807225 128.23741 4.05 -848.11507 -757.86264 0.071324545 -1786.5539 -1333.6271  810 -1333.6271 12.807225 128.2374 4.05 -848.08339 -757.84482 0.078273296 -1786.4836 -1333.6271  820 -1333.6271 12.807225 128.2374 4.05 -848.0853 -757.80564 0.069136475 -1786.5194 -1333.6271  830 -1333.6271 12.807225 128.2374 4.05 -848.09454 -757.78575 0.082848341 -1786.5807 -1333.6271  840 -1333.6271 12.807225 128.2374 4.05 -848.0851 -757.79929 0.078958088 -1786.535 -1333.6271  850 -1333.6271 12.807225 128.2374 4.05 -848.07775 -757.80563 0.076752431 -1786.5044 -1333.6271  860 -1333.6271 12.807225 128.2374 4.05 -848.08564 -757.79036 0.080355011 -1786.5469 -1333.6271  870 -1333.6271 12.807225 128.2374 4.05 -848.07696 -757.76979 0.077807288 -1786.5389 -1333.6271  880 -1333.6271 12.807225 128.2374 4.05 -848.05618 -757.76881 0.087736377 -1786.4875 -1333.6271  890 -1333.6271 12.807225 128.2374 4.05 -848.07882 -757.79982 0.082375704 -1786.519 -1333.6271  900 -1333.6271 12.807225 128.23741 4.05 -848.0994 -757.81515 0.084689319 -1786.5678 -1333.6271  910 -1333.6271 12.807225 128.23741 4.05 -848.09803 -757.82469 0.081802406 -1786.5512 -1333.6271  920 -1333.6271 12.807225 128.2374 4.05 -848.08577 -757.83065 0.081513649 -1786.5082 -1333.6271  930 -1333.6271 12.807225 128.2374 4.05 -848.08556 -757.83074 0.088823496 -1786.5148 -1333.6271  940 -1333.6271 12.807225 128.23741 4.05 -848.10457 -757.827 0.082734897 -1786.5695 -1333.6271  950 -1333.6271 12.807225 128.23741 4.05 -848.10677 -757.81386 0.090760075 -1786.5972 -1333.6271  960 -1333.6271 12.807225 128.23741 4.05 -848.12005 -757.83066 0.073178543 -1786.6027 -1333.6271  970 -1333.6271 12.807225 128.23741 4.05 -848.1237 -757.84763 0.077487755 -1786.601 -1333.6271  980 -1333.6271 12.807225 128.23742 4.05 -848.13818 -757.86007 0.069035121 -1786.6235 -1333.6271  990 -1333.6271 12.807225 128.23742 4.05 -848.14174 -757.84967 0.060986146 -1786.6365 -1333.6271  1000 -1333.6271 12.807225 128.23742 4.05 -848.13083 -757.82724 0.064474734 -1786.6297 -1333.6271  1010 -1333.6271 12.807225 128.23742 4.05 -848.13777 -757.83149 0.054251497 -1786.6361 -1333.6271  1020 -1333.6271 12.807225 128.23742 4.05 -848.14768 -757.84811 0.057927727 -1786.6528 -1333.6271  1030 -1333.6271 12.807225 128.23742 4.05 -848.15904 -757.86682 0.064362615 -1786.6747 -1333.6271  1040 -1333.6271 12.807225 128.23742 4.05 -848.1618 -757.87118 0.059115422 -1786.6733 -1333.6271  1050 -1333.6271 12.807225 128.23742 4.05 -848.14039 -757.85592 0.06793527 -1786.6332 -1333.6271  1060 -1333.6271 12.807225 128.23741 4.05 -848.11971 -757.85217 0.081008071 -1786.588 -1333.6271  1070 -1333.6271 12.807225 128.23741 4.05 -848.13593 -757.88672 0.081109667 -1786.6022 -1333.6271  1080 -1333.6271 12.807225 128.23742 4.05 -848.16566 -757.92725 0.090420596 -1786.6602 -1333.6271  1090 -1333.6271 12.807225 128.23742 4.05 -848.18418 -757.94318 0.098720416 -1786.7081 -1333.6271  1100 -1333.6271 12.807225 128.23742 4.05 -848.1711 -757.92067 0.089630981 -1786.6823 -1333.6271  1110 -1333.6271 12.807225 128.23741 4.05 -848.12905 -757.8823 0.089422736 -1786.5943 -1333.6271  1120 -1333.6271 12.807225 128.23741 4.05 -848.09903 -757.87537 0.093869076 -1786.5156 -1333.6271  1130 -1333.6271 12.807225 128.23741 4.05 -848.12665 -757.92993 0.08247581 -1786.5325 -1333.6271  1140 -1333.6271 12.807225 128.23742 4.05 -848.17393 -757.99436 0.078855615 -1786.6063 -1333.6271  1150 -1333.6271 12.807225 128.23742 4.05 -848.20306 -758.03028 0.089315911 -1786.6682 -1333.6271  1160 -1333.6271 12.807225 128.23742 4.05 -848.19524 -758.01621 0.086424058 -1786.6559 -1333.6271  1170 -1333.6271 12.807225 128.23742 4.05 -848.15668 -757.96957 0.077377595 -1786.5779 -1333.6271  1180 -1333.6271 12.807225 128.23741 4.05 -848.12107 -757.93229 0.078262218 -1786.5092 -1333.6271  1190 -1333.6271 12.807225 128.23741 4.05 -848.1351 -757.94709 0.071943603 -1786.5302 -1333.6271  1200 -1333.6271 12.807225 128.23742 4.05 -848.19734 -758.00988 0.00064058426 -1786.5828 -1333.6271  1210 -1333.6271 12.807225 128.23737 4.05 -847.86959 -757.7471 0.52900415 -1786.3907 -1333.6271  1220 -1333.6271 12.807225 128.23742 4.05 -848.19227 -757.98244 0.056925895 -1786.6513 -1333.6271  1227 -1333.6271 12.807225 128.23743 4.05 -848.24115 -758.01797 -0.018967943 -1786.6865 -1333.6271  Loop time of 4.04173 on 1 procs for 1227 steps with 398 atoms  94.3% CPU use with 1 MPI tasks x 1 OpenMP threads  Minimization stats:  Stopping criterion = energy tolerance  Energy initial, next-to-last, final =  -1333.62318020415 -1333.62711109752 -1333.62711109753  Force two-norm initial, final = 6.0977625 0.00011394522  Force max component initial, final = 6.0977625 7.8645698e-05  Final line search alpha, max atom move = 1.0000000 7.8645698e-05  Iterations, force evaluations = 1227 2453  MPI task timing breakdown:  Section | min time | avg time | max time |%varavg| %total  ---------------------------------------------------------------  Pair | 3.5653 | 3.5653 | 3.5653 | 0.0 | 88.21  Neigh | 0 | 0 | 0 | 0.0 | 0.00  Comm | 0.080508 | 0.080508 | 0.080508 | 0.0 | 1.99  Output | 0.0284 | 0.0284 | 0.0284 | 0.0 | 0.70  Modify | 0 | 0 | 0 | 0.0 | 0.00  Other | | 0.3676 | | | 9.09  Nlocal: 398.000 ave 398 max 398 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Nghost: 5167.00 ave 5167 max 5167 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Neighs: 27706.0 ave 27706 max 27706 min  Histogram: 1 0 0 0 0 0 0 0 0 0  FullNghs: 55436.0 ave 55436 max 55436 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Total # of neighbors = 55436  Ave neighs/atom = 139.28643  Neighbor list builds = 0  Dangerous builds = 0  # ---------- Calculate GB Energy ---------------------  variable minimumenergy equal -3.360000  variable esum equal "v\_minimumenergy \* count(all)"  variable xseng equal "c\_eatoms - (v\_minimumenergy \* count(all))"  variable gbarea equal "lx \* lz \* 2"  variable gbe equal "(c\_eatoms - (v\_minimumenergy \* count(all)))/v\_gbarea"  variable gbemJm2 equal ${gbe}\*16021.7733  variable gbemJm2 equal 0.0352124631661503\*16021.7733  variable gbernd equal round(${gbemJm2})  variable gbernd equal round(564.16610218266)  print "GB energy is ${gbemJm2} mJ/m^2"  GB energy is 564.16610218266 mJ/m^2  # ---------- Dump data into Data file -------------  reset\_timestep 0  dump 1 all cfg 10000 dump.al\_sig5\_310\_\*.cfg mass type xs ys zs c\_csym c\_eng fx fy fz  dump\_modify 1 element Al Al  minimize 1e-15 1e-15 5000 5000  WARNING: Using 'neigh\_modify every 1 delay 0 check yes' setting during minimization (src/min.cpp:188)  Per MPI rank memory allocation (min/avg/max) = 6.924 | 6.924 | 6.924 Mbytes  Step PotEng Lx Ly Lz Press Pxx Pyy Pzz c\_eatoms  0 -1333.6271 12.807225 128.23743 4.05 -848.24115 -758.01797 -0.018967943 -1786.6865 -1333.6271  10 -1333.6271 12.807225 128.23743 4.05 -848.23303 -758.03164 -0.0037472753 -1786.6637 -1333.6271  20 -1333.6271 12.807225 128.23743 4.05 -848.25105 -758.04599 -0.023085595 -1786.6841 -1333.6271  Loop time of 0.075799 on 1 procs for 20 steps with 398 atoms  61.8% CPU use with 1 MPI tasks x 1 OpenMP threads  Minimization stats:  Stopping criterion = energy tolerance  Energy initial, next-to-last, final =  -1333.62711109753 -1333.62711110309 -1333.62711110309  Force two-norm initial, final = 0.00011401525 0.00012714146  Force max component initial, final = 7.8747134e-05 9.5841936e-05  Final line search alpha, max atom move = 1.0000000 9.5841936e-05  Iterations, force evaluations = 20 40  MPI task timing breakdown:  Section | min time | avg time | max time |%varavg| %total  ---------------------------------------------------------------  Pair | 0.060979 | 0.060979 | 0.060979 | 0.0 | 80.45  Neigh | 0 | 0 | 0 | 0.0 | 0.00  Comm | 0.00099707 | 0.00099707 | 0.00099707 | 0.0 | 1.32  Output | 0.0016398 | 0.0016398 | 0.0016398 | 0.0 | 2.16  Modify | 0 | 0 | 0 | 0.0 | 0.00  Other | | 0.01218 | | | 16.07  Nlocal: 398.000 ave 398 max 398 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Nghost: 5167.00 ave 5167 max 5167 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Neighs: 27706.0 ave 27706 max 27706 min  Histogram: 1 0 0 0 0 0 0 0 0 0  FullNghs: 55412.0 ave 55412 max 55412 min  Histogram: 1 0 0 0 0 0 0 0 0 0  Total # of neighbors = 55412  Ave neighs/atom = 139.22613  Neighbor list builds = 0  Dangerous builds = 0  undump 1  write\_restart restart.al\_sig5\_310\_stgb  System init for write\_restart ...  print "All done"  All done  Total wall time: 0:00:06 |

1. **After calculation, GB Energy was found to be the value 564.16610218266 mJ/m2 in the log file.**

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| <https://drive.google.com/file/d/1flL_xiamqd4nFaCW2QOW2LMzL2FIIhvj/view?usp=sharing> |