Exercise

1. Calculate C44 according to Hooke’s law. (Hint: see the C11 and C12 scripts, change the region block to prism and change the direction of applied strain and calculated stress.
2. Calculate C11, C12, C44 and B (bulk modulus) of Ni by a different potential. Use this potential: **Y. Mishin, D. Farkas, M.J. Mehl, and D.A. Papaconstantopoulos, "Interatomic potentials for monoatomic metals from experimental data and ab initio calculations," Phys. Rev. B 59, 3393 (1999). DOI:**[**10.1103/PhysRevB.59.3393**](http://dx.doi.org/10.1103/PhysRevB.59.3393)  (Hint: to use this potential, change the pair\_style and pair\_coeff commands to these formats: pair\_style eam/alloy and pair\_coeff \* \* Ni99.eam.alloy Ni)