Stress formulation in the all-electron full-potential linearized augmented plane wave method NAOYUKI NAGASAKO, Toyota Central R&D labs., Inc., TAMIO OGUCHI, ISIR, Osaka University — Stress formulation in the linearlized augmented plane wave (LAPW) method has been proposed in 2002 [1] as an extension of the force formulation in the LAPW method [2]. However, pressure calculations only for Al and Si were reported in Ref.[1] and even now stress calculations have not yet been fully established in the LAPW method. In order to make it possible to efficiently relax lattice shape and atomic positions simultaneously and to precisely evaluate the elastic constants in the LAPW method, we reformulate stress formula in the LAPW method with the Soler-Williams representation [3]. Validity of the formulation is tested by comparing the pressure obtained as the trace of stress tensor with that estimated from total energies for a wide variety of material systems. Results show that pressure is estimated within the accuracy of less than 0.1 GPa. Calculations of the shear elastic constant show that the shear components of the stress tensor are also precisely computed with the present formulation [4].

[1] T. Thonhauser *et al.*, Solid State Commun. **124**, 275 (2002).
[2] R. Yu *et al.*, Phys. Rev. B **43**, 6411 (1991).
[3] J. M. Soler and A. R. Williams, Phys. Rev. B **40**, 1560 (1989).
[4] N. Nagasako and T. Oguchi, J. Phys. Soc. Jpn. **80**, 024701 (2011).

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