

Bulk Modulus for Solid Molecular Tritium: *ab initio* approximation

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Results for the bulk modulus approximation of the solid molecular tritium were calculated by means of simulations with *ab initio* methods. The selected method does not take into account the beta decay of tritium and its effects on the solid properties. These properties, which were obtained by this methodology, have been tested on experimental data of hydrogen and deuterium [1]. With bulk modulus we calculate the speed of sound by getting information about the changes occurring in the solid phase and behavioural approaches by the equation of state for this system or more complex Deuterium-Tritium (DT), which is used as fuel in target of the systems Inertial Confinement Fusion. This work is presented as a step before to solid DT analysis and mechanical properties. In addition the atomic structure is studied for solid state molecular tritium, showing the transition phase of I to II in solid phase to temperatures of 15 K, this transition shows consistency with the results presented for hydrogen but with a shift in the pressure [2,3]

Reference

- [1] C.Guerrero, S. Cuesta-López and JM. Perlado. “Room temperature sound velocity for hydrogen and deuterium to 6 GPa to 25 GPa”, unpublished.
- [2] C.Guerrero, S. Cuesta-López, JM. Perlado. “Structural properties of hydrogen isotopes in solid phase in the context of inertial fusion target manufacturing”. Proceedings of the Seventh Conference on Inertial Fusion Sciences and Applications (IFSA 2011). EPJ Web of Conferences **59**, 16004 (2013) DOI: [10.1051/epjconf/20135916004](https://doi.org/10.1051/epjconf/20135916004)
- [3] C. Guerrero, S. Cuesta-Lopez and JM. Perlado “Ab initio molecular dynamics: Relationship between structural phases and the sound velocity in dense hydrogen”. Europhysics Letters **108**: 26001 (2014)