SFP 2011-0

Time - Resolved Thz Spectroscopy of Bismuth Films: Experiment and Theory

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Bismuth, a group-V element which crystallizes in the rhombohedral A7 structure, is a well-known semimetal, and the archetype of thermoelectric materials [1]. The electronic structure of this material has been studied for more than 60 years, and it is still of great interest nowadays because of its interesting properties caused by the importance of the spin-orbit coupling effect [2], and of the possibility of obtaining bismuth monolayers.

The electron dynamics of photoexicted bismuth generate a Drude response that evolves in time. In contrast to graphite, the plasma frequency of bismuth displays an initial increase and a subsequent decay, as shown in Fig. 1. These two regimes were still unexplained.

We have performed state-of-the-art *ab initio* calculations in the framework of the Density Functional Theory with the Generalized Gradient Approximation, using a plane wave basis set and the pseudopotential scheme, with the QUANTUM ESPRESSO package [3]. According to our calculations, the peculiar behaviour of the plasma frequency is due to the local minima present in the band structure: a substantial portion of the photoexicted electrons first thermalizes in these local minima, while it reaches the L point only 0.7 ps after photoexcitation. This yields the two regimes observed in the experiment.

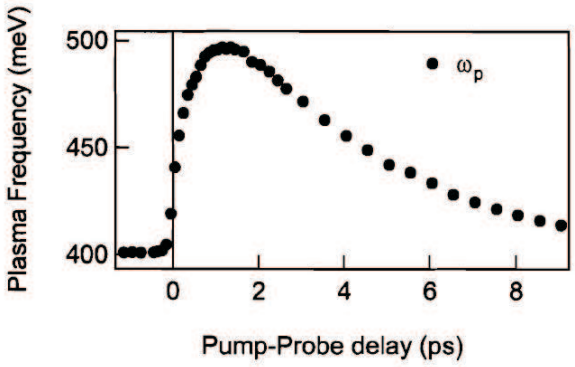

Fig. 1: *Pump-induced plasma frequency in bismuth*

Acknowledgments. IT gratefully acknowledges fruitful discussions with Andrea Dal Corso concerning a generation of the pseudopotential for bismuth.

Références

[1] J.P. Issi, "Low Temperature Transport Properties of the group V Semimetals", Aust. J. Phys. **32**, 585 (1979).

[2] X. Gonze, J.-P. Michenaud, and J.-P. Vigneron, "First-principles study of As, Sb, and Bi electronic properties", Phys. Rev. B **41**, 11827 (1990).

[3] P. Giannozzi *et al.*, "QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials", J. Phys. Condens. Matter **21**, 395502 (2009).