	Experiment title: Phonon dynamics and thermal transport in amorphous/crystalline nanocomposites: a microscopic insight onto the mechanisms at play	**Experiment number**: HC-4022
Beamline: ID18	**Date of experiment**: from: 09/09/18 to: 11/09/18	**Date of report**: 26/02/18
Shifts:	**Local contact(s)**:M. Mikolasek	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

V. M. Giordano*, M. Katsikini* and C. Maurizio*

Report:

Nanocomposites, made of (semi)conductive crystalline nanoinclusions embedded in an amorphous insulating matrix, have recently come at the forefront of materials research for energy harvesting applications, where thermal management represents a major challenge. Theoretical investigations have indeed demonstrated that phonon dynamics in such heterogeneous materials can be dramatically perturbed, and especially in presence of an elastic contrast between the two constituents, leading to a surprising reduction of the thermal conductivity, not predictable by any effective medium approach. While macroscopic measurements have been largely performed on these materials, a microscopic experimental investigation of phonon dynamics, fundamental for understanding the microscopic processes at play, is still missing. In this proposal we wanted to measure the vibrational density of states in nanocomposites made of Au and GaN nanoparticles embedded in amorphous silica, in order to explore the effects on the dynamics of different factors such as the elastic contrast between matrix and inclusions, the different nano-particles amount and size.

The requested beamtime was about 6 days, taking into acount especially the need of performing very large and long-counted energy scans due to the large range of the DOS of silica, and its low scattering rate.

The beamtime has been shortened to only 2 days, for beamtime lack. In such a short time we could not have performed our study and we could not have gotten not even a single answer to the three main questions of the project. At the same time, prior to this experiment, we finalized the analysis of HC3371 and complemented the phonon data with calculations and other measurements, on the system C-GeTe: nanograins of GeTe embedded in amorphous carbon. The appearance of a pseudo Boson Peak at about 3 meV in that system, increasing with the carbon content, suggests that a glass-like dynamics can be initiated in a nanocomposite with a majoritary crystalline component, by tuning the elastic heterogeneities. Still, we needed to be sure that it was not just an effect of the reduced grain size.

Face to the upcoming ESRF long shutdown, which would have made every partial measurement useless for years, in agreement with the beamline staff, we have thus given the priority to the measurement of a sample of pure nanocrystalline GeTe with a grain size comparable to the one in the C-GeTe nanocomposite, in order to complete our previous project.

To this aim, we have prepared two samples, nano-Gete with a grain size of 50 nm, with 100nm thickness and 1 micron thickness on Silicon substrate and measured them at 50K. The thinner sample corresponds to the one that we have completely characterized with electrical meaurements to assess the electronic contribution

to thermal conductivity, but it is more difficult for DOS measurements because of the possible signal contamination from the substrate. The second sample has been used then to confirm the data on the thinner one, as the substrate does not contribute.

Our results clearly show that the reduction of the grain size of GeTe from ~100nm in a standard thin film down to 30nm does not give origin to a pseudo-Boson Peak. Still, we could not prepare a sample with smaller grain size, and we note that in the nanocomposites the grain size is between 20 and 30 nm. The question remains if a further reduction could lead to such a phenomenology. Work is on-going for answering this question.

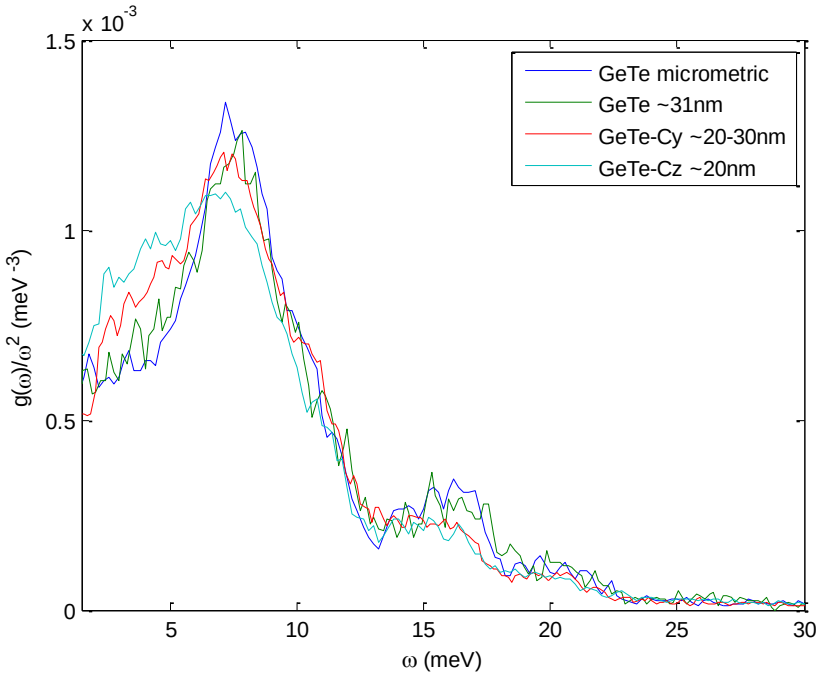

Figure 1: Reduced Density of states at 50 K of polycrystalline GeTe and C-doped GeTe after raw data reduction