

INELASTIC NEUTRON SCATTERING FROM AMORPHOUS $\text{Fe}_{40}\text{Zr}_{60}$ DOPED WITH DIFFERENT CONCENTRATIONS OF KRYPTON (0,1,7 at.%)

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Abstract.— By means of time-of-flight neutron inelastic scattering techniques we have obtained the generalized vibrational densities of states $G(\hbar\omega)$ of undoped polycrystalline and amorphous $\text{Fe}_{40}\text{Zr}_{60}$ and of amorphous samples doped with 1 and 7 at.% Kr. The amorphous compound displays a triangular shaped $G(\hbar\omega)$ which is very different from the strongly structured crystalline modification. Concerning the amorphous alloys, the energetic range of the additional Kr modes indicates that the Kr atoms are embedded in their host matrix as single atoms or perhaps small clusters and not as bubbles as was found in metals.

1. Experiment.— We have produced amorphous $\text{Fe}_{40}\text{Zr}_{60}$ undoped and doped with 1 and 7 at.% Kr using a triode sputtering system as described in /1/. The structure of our samples was checked by neutron diffraction. No Debye-Scherrer-lines were observed showing the amorphous state of the materials. By means of inelastic neutron scattering techniques from powder samples we determined the generalized vibrational densities of states $G(\hbar\omega)$. The experiments were carried out at the FR2 research reactor in Karlsruhe using the multidetector time-of-flight spectrometer TOF II. The incident neutron energy was 5 meV, the 60 He^3 -counters covered scattering angles between 80 and 166 degrees.

To crystallize the alloy we heated an amorphous sample up to about 700°C in UHV. Neutron diffraction revealed that the material had completely crystallized. The largest amount had transformed to FeZr_2 a tetragonal CuAl_2 (C16)-type structure /2/ but also minor parts of other phases were present.

2. Results and discussion.— In Fig. 1 we show the time-of-flight distribution (background subtracted) of three amorphous $\text{Fe}_{40}\text{Zr}_{60}$ alloys containing 0-1 and 7 at.% krypton. Towards smaller energy transfers we register a strong enhancement of intensity with rising Kr concentration. In fact even the sample doped with 1 at.% Kr already shows a well defined increase. From these scattering data the generalized vibrational densities of states were deduced. They are shown in Fig. 2 together with $G(\hbar\omega)$ after crystallization of the undoped alloy. Amorphous undoped $\text{Fe}_{40}\text{Zr}_{60}$ has a triangular frequency distribution which peaks around 20 meV and extends to 40 meV. Astonishing is the fact that there is no Debye like behaviour in $G(\hbar\omega)$ down to our experimental limit of 1 meV. This shape of $G(\hbar\omega)$ is very different from the phonon density of states curve of the crystalline modification where a pronounced decrease

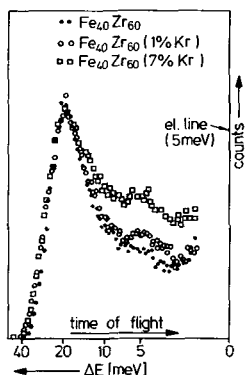


Fig. 1: Time-of-flight spectra of amorphous Fe₄₀Zr₆₀ with different Kr concentrations

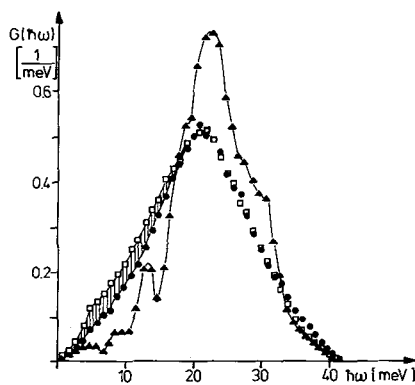


Fig. 2: Comparison of the vibrational densities of states of crystalline Fe₄₀Zr₆₀ ▲-▲ with that of the amorphous alloy: ●-● undoped, □-□ doped with 7 at.% Kr

of intensity is registered below 17 meV with a dip at 6.5 meV and a rather sharp peak at 13 meV. The maximum of $G(\hbar\omega)$ is shifted to higher energies and now centers around 23 meV while the cut-off frequency remains the same i.e. 40 meV.

Amorphous Fe₄₀Zr₆₀ with 7 at.% Kr exhibits additional intensities from 1 meV up to 20 meV with a maximum of 10 meV. From scattering power considerations these modes have been attributed to the Kr atoms i.e. one expects an intensity gain of approximately 5% for the doped sample which is nicely confirmed. For solid Kr the frequency spectrum ends at 6 meV /3/ whereas we obtained a much harder Kr spectrum which is shown in Fig. 3. From this we conclude that the force constants between Kr and the

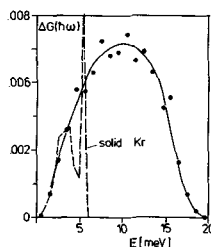


Fig. 3: The Kr vibrations in amorphous Fe₄₀Zr₆₀

transition metal atoms must be about 10 times larger than the forces in solid Kr. If Kr was enclosed in its host matrix in the form of bubbles it would be in its liquid state due to its critical temperature. As the dynamical forces then were of the Van de Waals type they would be even weaker than for the solid state. From this we conclude that the Kr-atoms are embedded as single atoms or at most as very small clusters in the amorphous host matrix.

- References.- /1/ H.-J. Schmidt, E. Henrich, T. Fritsch, F. Gompf, B. Renker, E. Mohs, Proc. of the Int. Conf. on Liquid and Amorphous Metals, Grenoble 1980
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