

of the curvature leads to the increasing of the amplitude of the diffracted and weakly absorbed field and simultaneous decreasing of the amplitudes of diffracted and strongly absorbed field as well as amplitude of both passing fields. With increasing the curvature of the reflecting atomic planes, the energy transferred to the diffracted weakly absorbed field is increases. There is a certain value of the curvature for which the total energy is transmitted only to this field. As a consequence the absorption coefficient of the crystal is sufficiently decreases. The further increasing of the curvature leads to decreasing of the energy transferred to the diffracted weakly absorbed field (the absorption coefficient is increased again). In order to explain the above-mentioned processes the total intensity of passed and diffracted beams in the region of Darwin's table are analysed at different curvatures of reflecting atomic planes. It is shown that with decreasing the radius of curvature the total intensity at exactly Bragg angle and over all region of Darwin's table is increased, i.e. the absorption coefficient is decreases. Theoretical calculations have been carried out for a quartz single crystal for several families of reflecting atomic planes. However the above-mentioned effect was most obviously manifested for (10-11) family of reflecting planes.

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Crystallography of CuZnAl Austenite via Combined XANES, EXAFS and XRD Analysis.

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Shape memory alloys (SMAs) belong to the class of smart materials (together with ferroelectric, piezoelectric, etc.) since they underscore a reversible variation in macroscopic size driven by changes of external conditions (temperature, pressure, or magnetic field). SMAs can be as consequence employed in the manufactory of actuators controlled by one of these external parameters and, viceversa, in the design of sensors. SMAs have several applications in the field of engineering and medical science: tube coupling, active endoscopes, and artificial muscle components for robotics. The shape memory behavior is due to a displacive phase transition (martensitic) which takes place in different metals. This transformation is a cooperative phenomenon (like

ferromagnetism) which, despite the small displacement of the single atoms, results in a macroscopic shape variation since all atoms move in the same direction into a domain. We have investigated and solved the structure of the parent phase (austenite) of the martensitic transition in CuZnAl shape memory alloys by a combined X-ray absorption (EXAFS, XANES) and diffraction analysis [1], taking advantage of the different length scale sensitivity of the two techniques. Ab-initio simulations of the near Zn-edge X-ray absorption coefficient (XANES) allow us to directly discard the hypothesis of a DO₃ superstructure. At the same time, we give evidence of the existence of an ordered structure (B2-like) different from the L2₁, one recently proposed by neutron diffraction [2]. However, some partial L2₁ ordering is present at room temperature: this superstructure develops and recovers order when increasing the temperature above 400 K. Note that DO₃ and L2₁ phases differ only for the relative site occupancy by Zn and Cu atoms, indeed they cannot be discriminated by the sole X-ray diffraction, due to the close atomic number of the two elements. The formation of either B2-like or L2₁ superstructures has an important effect on the martensitic transition temperature. Our work presents a typical example in which X-ray Absorption can be used for crystallographic phase determination when the very similar X-ray scattering factors of the elements present in the alloy makes some ordering configurations invisible to X-ray diffraction only. The same method can be applied in the study of other intermetallic compounds.

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