Title: Investigation of vacancies in Fe-Al alloys

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Abstract: Fe-Al alloys exhibit relatively high vacancy concentrations, which significantly influence the mechanical properties of these alloys. Positron annihilation spectroscopy was employed for investigations of vacancies in this work and the vacancy concentrations in Fe-Al alloys were determined by positron lifetime spectroscopy and measurements of positron diffusion length of implanted monogenergetic positrons. The correlation of hardness with the vacancy concentration was characterized by determination of the vacancy hardening coefficient in Fe-Al alloys. The thermal evolutions of hardness and the vacancy concentration were compared during the annealing of the Fe-Al alloys with various compositions. Coincidence Doppler broadening of annihilation peak was employed for determination of the chemical composition of quenched-in vacancies in Fe-Al alloys. Increased concentration of Al atoms in surrounding vacancies in Fe-Al alloys was related to the attractive interaction between the Al atoms and the vacancy. Quantum mechanical *ab initio* calculations were performed in order to explain the measured positron annihilation characteristics in Fe-Al alloys. Ionic relaxations of the atoms surrounding vacancies were found to have significant effect on the lifetime of positrons trapped at vacancies. Inclusion of ionic relaxations into the calculations of positron lifetimes significantly improved the agreement of the calculated lifetimes with experiment.

Keywords: Fe-Al alloys, intermetallics, vacancies, positron annihilation