Atomic disordering effects in the electronic structure of zircon: Spectroscopic studies and *ab initio* calculations

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The electronic structures of crystalline and radiation damaged zircon crystals have been investigated using the combination of photoluminescence spectroscopy with selective excitation by synchrotron (HASYLAB, DESY) irradiation (soft X-ray and visible range) and X-ray emission spectroscopy. The series of natural crystalline and partially metamict samples from the Urals and Yakutiya (Russia) before and after annealing (up to 1500 K) were used. The computer calculations of the electronic structures of intrinsic defects and metamict areas in zircon were performed with the use of *ab initio* quantum-chemical cluster method of X_α discrete variation.

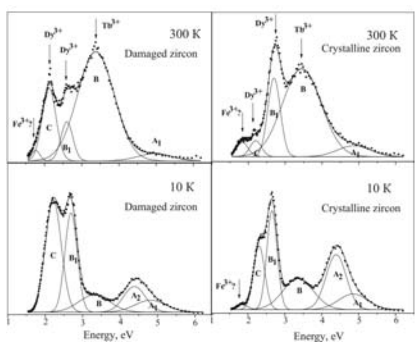

Figure 1: Luminescence spectra of crystalline and damaged zircon crystals at the excitation energy 6.9 eV.

The luminescence bands of initial and annealed zircon crystals (Fig.1) were divided into two groups: defect bands (C,B,B_1) and intrinsic bands (A_1,A_2). The excitation spectra of intrinsic luminescence near the fundamental edge (7.1 eV) and X-ray emission spectra Si K_β were used for the revealing the peculiarities of electronic structure for crystalline and damaged zircon. The electronic structure and chemical bonding (effective atomic charges, energy and spatial electron density distributions) of crystalline and disordered zircon were calculated.

Magmatic evolution of granites from Shir-Kuh area, Yazd block, Central Iran: anatexis of deep crustal rocks

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The peraluminous, calc-alkaline, S-type granite of Shir-Kuh in Central Iran is intrusive into Lower Jurassic sandstones and shales. Combined petrography, chemistry/ mineralogy and whole-rock geochemistry indicates that fractional crystallization was very effective differentiation process during formation and emplacement of the batholith. The crystallization sequence has three main stages represented by the granodiorite, monzogranite and leucogranite facies. The monzogranite facies are a differentiated melt from a parental magma due to removal of material in the granodiorites. It is consistent with plagioclase accumulation and crystallization of biotite in the granodiorites. The leucogranites represent a late residual melt after total crystallization of the monzogranite facies. The parental magma of the Shir-Kuh granite was derived from a plagioclase-rich metasedimentary source (metagreywacke) in the middle crust (~ 19-20 km) under moderate-low magmatic temperature conditions.

The structural and geochemical data suggest that the Shir-Kuh granitic batholith formed in a volcanic arc setting which consistent with subduction of the Neotethys oceanic crust beneath the Central Iranian microcontinent in Jurassic time