The exchange splitting of surface and bulk electronic states in excited magnetic states of Gd.

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Recent pump-probe experiments provide time evolution of the bulk and surface electronic states in Gd exited by the laser pulse. These new experiments are in close connection with earlier spectroscopic experiments probing temperature dependence of the exchange splitting of the bulk and surface states. The two types of electronic states show very different behavior. Most of the researchers suggest to treat the bulk states within a Stoner model whereas the surface states show clear non-Stoner behavior and remain exchange-split above the Curie temperature. We report first-principles study of the electronic states in both thermally excited Gd and Gd subjected to the laser irradiation. We model the excited states of the system by the noncollinearity of the 4f spin moments where stronger excitations correspond to larger noncollinearity of the neighboring 4f moments. We provide arguments for ultra-fast character of the 4f-moments disordering by hot electrons and discuss the possible ways of the treatment of the induced 5d6s moments. In agreement with experiments we obtained strong difference in the dynamics of the bulk and surface states. We apply the concept of spin-mixing to characterize the electronic states of the excited system. The surface states remain weakly spin-mixed with respect to the local atomic spin axes that explains the presence of the exchange splitting in highly excited systems. On the other hand the bulk states are strongly spin-mixed with respect to the local atomic axes and average the influence of the atomic spin-up and spin-down potentials. This results in the properties that are usually associated with the Stoner model. We analyze quantitatively the dynamics of the electronic states and compare the numerical results with the results of the recent experiment.