Name	**Akimasa Sakuma**
Organization	**Tohoku University**
Division/Department	**Department of Applied Physics, Graduate School of Engineering,**
Title	**Prof. Dr.**

Presentation Title

First principles calculation of the Gilbert damping for transition metal alloys and Heusler alloys

Abstract

Much interest has been paid on controlling the magnetic damping in the magnetic devices such as magnetic recording system, MRAM, and some other spintronics applications. This stimulates the intensive studies on the microscopic origin of magnetic damping of magnetic materials. Theoretically, Kambersky[1)] and Gilmore et al.[2)] (K-G) proposed a quantitative method to calculate the Gilbert damping coefficients based on the first principles technique for the electronic structure. Basic concept of this theory corresponds to ones describing the relaxation time (T_1, T_2) of NMR measurements, and then the damping coefficient is expressed as a correlation function of torques acting on the spins in the following form

$$\alpha = -\frac{1}{2S}\lim_{\omega\to 0}\frac{1}{\omega}\mathrm{Im}\,\Pi(\omega), \quad \Pi(\omega) = -i\int_0^\infty dt\, e^{i\omega t}\langle[\Gamma^+(t),\Gamma(0)]\rangle \qquad (1)$$

Here, S represents expectation value of the spin and Γ is a torque operator acting on spins whish is expressed by $\Gamma = (1/\hbar)[S_-, H_{SO}]$ where H_{SO} is the spin-orbit interaction Hamiltonian of the electronic system and $S_- \equiv S_x - iS_y$. K-G evaluated the Gilbert damping constants α of Fe and Ni metals including phenomenological relaxation time of electrons. It should be noted that in the presence of intrinsic spin flip processes due to spin-orbit interaction, Gilbert damping diverges in the absence of electron scattering due to impurities or defects. Furthermore, diagrammatic technique predicts that only the magnetic scattering has an influence on α, while non-magnetic scattering does not.[3)] In this sense, the treatment by

K-G is semi-empirical, and therefore more quantitative approach is desired to deal with realistic materials including disordering, impurities and defects.

In the present work, we have developed the calculation method of α based on eq. (1) for substitutional disordered alloys such as $Fe_{1-X}Co_X$, $Fe_{1-X}Ni_X$ and some Heusler alloys with partial disorder which are expected to be spintronics materials. The use is made of the coherent potential approximation (CPA) in the tight-binding linear muffin-tin orbital (TB-LMTO) method within the framework of the density functional theory. Similar approach using the Koringa-Kohn-Rostocker (KKR) method has recently been proposed by Brataas et al.[4] and Ebert et al.[5], but in their equation $\Gamma = (1/\hbar)[S_-, H_{SO}]$ is replaced by $\Gamma = (1/\hbar)[S_-, H_{exch}]$ where H_{exch} represents the exchange splitting energy due to the molecular field. It should be noted that the magnitudes of their coupling constant are much different each other. In this work, we will discuss the relationship between these two approaches.

References

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