# Evaluation of Spin Lifetime in Thin Silicon Films by Multilevel Parallelization

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To evaluate the spin relaxation time in silicon films, multi-dimensional integrals over the subband electron momenta before and after scattering must be evaluated. The electron-phonon and surface roughness spin relaxation matrix elements describing the spin-flip scattering events are computed numerically by using accurate subband wave functions which are obtained with the help of a two-band **k·p** method with the intrinsic spin-orbit interaction included [1]. Because of the spin relaxation hot spots, the scattering matrix elements are characterized by very narrow and sharp peaks [1], which must be properly resolved by using an appropriately fine mesh in the **k**-space. In order to evaluate the multi-dimensional integrals, the scattering matrix elements are computed numerically at approximately a billion points. Because of the limited memory per node, a straightforward MPI-based evaluation of the spin relaxation time by using adaptive integration techniques is prohibitively time-consuming, and a different parallelization approach has to be applied. In order to overcome the limitations, a two-stage parallelization scheme is realized. At the first stage all static wave function and energy data are calculated and archived in a binary file as a file-based cache technique which requires about 7GB for one stress point with high accuracy. At the second stage the spin lifetime is calculated by loading and using these data in cache memory. At each stage the computation is performed in parallel. We have analyzed and optimized the memory and computation time requirements for different parallelization configurations by employing a hybrid MPI-OpenMP approach. We found that the first pre-calculation step (first stage) is best performed with a pure MPI scheme. The second stage demands large data to be stored and used in cache memory, and hence the spin relaxation calculations are efficiently performed by a hybrid MPI-OpenMP approach because of the memory demands.

This approach has been tested on the Vienna Scientific Cluster [2] using 416 cores. Only 40 minutes for a single relaxation time data point (around 300 core-hours) are required. By employing this parallelization technique we have shown that shear strain enhances the spin lifetime in thin silicon films by orders of magnitude, and that the spin injection orientation also has an impact.

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[1]. V. Sverdlov and S. Selberherr, Physics Reports 585, pp. 1-40 (2015).

[2] Vienna Scientific Cluster: http://www.vsc.ac.at/systems/vsc-2/.