Calculation of Dopant Concentration Profiles from Grazing Emission X-Ray Fluorescence Measurements

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In semiconductor technology it is of great importance to know the concentration profiles of Group III or Group V dopant elements in silicon wafers. Several techniques are available to determine the dopant concentration as a function of depth, and each technique has its own advantages and disadvantages. We mention Secondary Ion Mass Spectrometry (SIMS), which has the disadvantage of being destructive and of being unreliable for shallow concentration profiles. Another technique is Rutherford Backscattering Spectrometry (RBS). This technique is not destructive but has the drawback that only relatively high concentrations of dopants can be detected.

A new, nondestructive, technique for determining shallow concentration profiles of dopants, which uses Grazing-Emission X-Ray Fluorescence (GEXRF) spectrometry is discussed. In this type of X-ray spectrometry the doped silicon wafer is irradiated by a polychromatic conventional X-ray tube and the emitted fluorescence intensity is detected at grazing angles to the surface of the silicon wafer. A double slit collimator is used to select the emission angles and a crystal monochromator selects the wavelength.

The measured fluorescence intensity as a function of the emission angle can be expressed in terms of the dopant concentration as a function of depth. This expression is an integral equation which can be considered a truncated Laplace transform. The dopant concentration can be obtained by inverting this integral equation. Although the dopant concentration is uniquely determined by an angle scan of the fluorescence intensities, the inversion is ill-posed; this means that the computed concentration is extremely sensitive to small errors in the measurements. Therefore, it is not attempted to invert the truncated Laplace transform directly. Instead, because the

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eigenfunctions of the Laplace transform are explicitly known, the Laplace transform can be diagonalized. The diagonalized form clearly demonstrates the ill-posedness of the inversion problem.

In order to stabilize the inversion so-called regularization methods are used. Two of them are discussed. The first one is Tikhonov regularization, which can be formulated in terms of the singular value decomposition of the integral operator; the second one is the maximum entropy regularization. The main emphasis is layed on applying the maximum entropy method to solve the ill-posed problem of inverting the truncated Laplace transform. Existence and convergence of the regularized solution can be proved.

The Tikhonov regularization method is compared to the maximum entropy method by performing several numerical experiments involving the inversion of the truncated Laplace transform. It is found that the extrapolation of measured data, which is needed in Tikhonov's regularization, forms the main limitation of this method. Furthermore, the maximum entropy method is found to perform better for steep concentration profiles. However, Tikhonov's method requires much less CPU time than the maximum entropy method.