Mechanical Reliability of Piezoelectric Microelectromechanical Systems Pb[(Zr_{0.52}Ti_{0.48})_{0.98}Nb_{0.02}]O₃ Films

K. Coleman^{1*}, J. Walker¹, H.G. Yeo¹ and S. Trolier-McKinstry¹

¹Materials Science and Engineering Dept. & Materials Research Institute, Pennsylvania State University N-225 Millennium Science Complex, University Park, PA, 16802, USA *Kathleen Coleman: kpc8@psu.edu

Piezoelectric Microelectromechanical systems (PiezoMEMS) are used in sensors, actuators, and energy harvesting devices. In all of these applications, the mechanical reliability of the bending structures is critical. However, relatively little is known about either the mechanical reliability or the coupling between electrical and mechanical failure modes. Therefore, understanding the controlling mechanisms of the electric field and mechanical strain limits of the $Pb[(Zr_{0.52}Ti_{0.48})_{0.98}Nb_{0.02}]O_3$ (PZT) films is critical for a broader use of these films in piezoMEMS applications.

The PZT films studied were prepared either through RF sputtering or chemical solution deposition. 50 μ m thick Ni foils were used as flexible substrates; a protective buffer barrier of HfO₂ was needed to prevent oxidation of the substrate. In addition to Ni foils, Si substrates were also used to establish the effect of the substrate choice on the reliability of these films. The LaNiO₃ (LNO), bottom electrode was deposited by chemical solution deposition with strong (100) orientation. The thickness of the PZT films was varied from 500 nm, 1 μ m, to 2 μ m; all films have a preferred {100} orientation. Films on Si had remanent polarizations $\geq 20 \ \mu$ C/cm². The higher compressive strain in the PZT films on Ni led to higher remanent polarizations.

In addition, the direct effective transverse piezoelectric coefficient, $e_{31,f}$ was studied as a function of compressive strain. As the compressive strain increased, the hysteresis curve rotates counterclockwise and so the sample has a higher remanent polarization. It was found that the magnitude of $e_{31,f}$ increased as a result of the compressive strain. On Si, the maximum compressive strain reached in the PZT film was $5x10^{-4}$. This was limited by the brittle nature of the Si substrate, which failed under tension due to the beam bending. PZT films on Ni foils reached a maximum compressive strain of approximately $5x10^{-3}$. At this strain, the PZT 1µm film cracked and delaminated. Thus, for devices which require large maximum strains (such as energy harvesters), Ni foil substrates are preferred.

The magnitude of $e_{31,f}$ depends on the applied DC electric field. The $e_{31,f}$ increased up to the coercive field, even in poled films, because of the improved alignment of the dipoles in the film. Beyond the coercive field, the $e_{31,f}$ decreased, presumably due to a decrease in the extrinsic contributions and a dielectric stiffening effect at the high fields. Dielectric breakdown was induced in the films by applying DC electric fields up to ten times the coercive field for periods of up to 10 minutes and correlation between thermal and mechanical breakdown events were studied. Thermal and mechanical breakdown events showed varying degrees of correlation. Thermal breakdown events tend to initiate local mechanical failure, initiating cracks. These local mechanical failures were seen to link thermal breakdown events, indicating that cracking may initiate subsequent thermal breakdown events. The degree of this thermal and mechanical breakdown sites were highly correlated, while films on Ni foil substrates exhibited a significant decrease in the occurrence of correlated breakdown events. It is believed that this may be due to the improved thermal conductivity of the Ni, relative to the Si.