

Tusche *et al.* Reply: The magnetoresistance (MR) of planar tunnel junctions is determined essentially by properties of the interfaces. As Velev, Belashchenko, and Tsymbal correctly point out in the preceding Comment [1] on our Letter [2], interface resonances can lead to a huge MR since they provide highly efficient transmission channels in one of the magnetization configurations, typically in the parallel (P) configuration. This is nicely demonstrated by the calculations reported in the Comment and in the Refs. [3,4]. We would like to point out that the huge tunneling magnetoresistance (TMR) found in our calculations (MR >7000%) has the same origin. Thus, we are very pleased by the fact that these calculations fully confirm our results.

In our Letter we have studied how symmetric and asymmetric interfaces between electrodes and a barrier can affect the MR in Fe/MgO/Fe(001). We have shown that in the case of symmetric ideal interfaces the TMR ratio increases continually with the number of MgO layers, while in the asymmetric configuration it is destroyed by the mismatch of resonant states. This effect can be clearly seen in Fig. 1, where k_{\parallel} -resolved transmissions in the full two-dimensional Brillouin zone (2BZ) are presented for Fe/(MgO)₄/Fe(001). The conductance of the tunnel junction is proportional to the 2BZ integral of the transmission.

With the ideal symmetric interfaces (upper panels) the conductance in the P configuration (panel a) is strongly enhanced, and in the antiparallel (AP) configuration

(panel b) it is reduced, explaining thereby the huge TMR ratio [5]. In the case of asymmetric interfaces, the conductance in the P configuration decreases dramatically (panel c), while the conductance in the AP case (panel d) increases, so leading to a negative TMR ratio [4]. Thus, in the parallel configuration a huge MR occurs if interface resonances are present at both interfaces at the same energy and at the same wave vector. Hence, a mismatch in either energy or wave vector destroys this “handshake” and can reduce the MR considerably. Therefore, the MR typically drops when applying a bias voltage [6,7] or upon structural disorder, the latter introducing diffusive scattering [3,4].

That both effects reduce the MR is also shown by calculations of Velev *et al.* [1]. In their calculations structural disorder is treated by introducing a uniform finite lifetime of the scattering channels. However, the reduction of the lifetime is expected to be strongly k_{\parallel} and energy dependent, as is well known from electronic-structure calculations for alloys. Nevertheless, the calculations of Velev *et al.* provide a useful qualitative understanding.

For a quantitative study on how structural disorder influences the TMR amplitude, more sophisticated ways to consider disorder have to be invoked. This could be achieved either by using a supercell approach or by applying the coherent potential approximation. Such calculations, although very demanding, would be very helpful, in particular, for the case of the partially occupied FeO_x layers in Fe/MgO/Fe tunnel junctions.

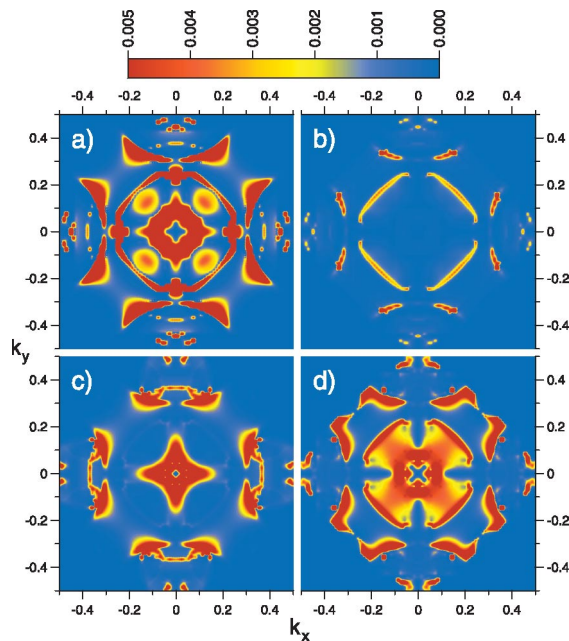


FIG. 1 (color). Calculated k_{\parallel} -resolved transmission in the 2BZ for symmetric Fe-FeO-MgO-FeO-Fe (upper panels) and asymmetric Fe-MgO-FeO-Fe (lower panels) magnetic tunnel junctions with four MgO layers. Panels (a) and (c), refer to the P configuration, panels (b) and (d), to the AP configuration. Wave vectors k_x and k_y are given in reciprocal lattice units.

C. Tusche,¹ H. L. Meyerheim,¹ N. Jedrecy,² G. Renaud,³

A. Ernst,¹ J. Henk,¹ P. Bruno,¹ and J. Kirschner¹

¹Max-Planck-Institut für Mikrostrukturphysik
Weinberg 2, D-06120 Halle, Germany

²Institut des NanoSciences de Paris
Université Paris 6 et 7
et CNRS-UMR 7588

4 place Jussieu,
F-75252 Paris Cedex 05, France

³CEA-Grenoble
17 rue des Martyrs
F-38054 Grenoble, France

Received 10 January 2006; published 21 March 2006

DOI: [10.1103/PhysRevLett.96.119602](https://doi.org/10.1103/PhysRevLett.96.119602)

PACS numbers: 68.35.Ct, 61.10.-i, 75.70.Ak

- [1] J.P. Velev, K.D. Belashchenko, and E.Y. Tsymbal, preceding Comment, Phys. Rev. Lett. **96**, 119601 (2006).
- [2] C. Tusche *et al.*, Phys. Rev. Lett. **95**, 176101 (2005).
- [3] K.D. Belashchenko, J. Velev, and E.Y. Tsymbal, Phys. Rev. B **72**, 140404(R) (2005).
- [4] X.-G. Zhang, W.H. Butler, and A. Bandyopadhyay, Phys. Rev. B **68**, 092402 (2003).
- [5] W.H. Butler, X.-G. Zhang, T.C. Schulthess, and J.M. MacLaren, Phys. Rev. B **63**, 054416 (2001).
- [6] C. Zhang *et al.*, Phys. Rev. B **69**, 134406 (2004).
- [7] C. Heiliger, P. Zahn, B. Yu. Yavorsky, and I. Mertig, Phys. Rev. B **72**, 180406(R) (2005).