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EDITORIAL

Focus on the Rashba effect

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Abstract

The Rashba effect, discovered in 1959, continues to supply fertile ground for fundamental research and applications. It provided the basis for the proposal of the spin transistor by Datta and Das in 1990, which has largely inspired the broad and dynamic field of spintronics. More recent developments include new materials for the Rashba effect such as metal surfaces, interfaces and bulk materials. It has also given rise to new phenomena such as spin currents and the spin Hall effect, including its quantized version, which has led to the very active field of topological insulators. The Rashba effect plays a crucial role in yet more exotic fields of physics such as the search for Majorana fermions at semiconductor-superconductor interfaces and the interaction of ultracold atomic Bose and Fermi gases. Advances in our understanding of Rashba-type spin-orbit couplings, both qualitatively and quantitatively, can be obtained in many different ways. This focus issue brings together the wide range of research activities on Rashba physics to further promote the development of our physical pictures and concepts in this field. The present Editorial gives a brief account on the history of the Rashba effect including material that was previously not easily accessible before summarizing the key results of the present focus issue as a guidance to the reader.

The importance of spin-orbit (SO) coupling for the band structure of Bloch electrons was first noted by Elliott [1, 2] and Dresselhaus *et al* [3]. Elliott [2] pointed out that we obtain (at least) a two-fold spin degeneracy of the energy bands $E_n(\boldsymbol{k})$ for each wave vector $\boldsymbol{k}$ throughout the Brillouin zone if space inversion is a good symmetry of the crystal structure. Dresselhaus *et al* [3] (see also [4]) demonstrated that the SO splitting of the atomic p orbitals may qualitatively alter cyclotron resonance spectra in silicon and germanium.

Using group theory, Dresselhaus [5] studied the effect of SO coupling on semiconductors with the inversion asymmetric zincblende structure, which is the crystal structure of many III-V and II-VI semiconductors such as GaAs, InSb, and CdTe (see also [6]). He predicted an anisotropic spin splitting of the dispersion $E(\boldsymbol{k})$, cubic in the wave vector $\boldsymbol{k}$ for bands with symmetry Γ_6, which became known as 'Dresselhaus SO splitting'.

The second important crystal structure besides zincblende, realized by many III-V and II-VI semiconductors is the likewise inversion asymmetric wurtzite structure (e.g., GaN, CdS, and ZnO). In 1959 Rashba published two papers on the 'Symmetry of Energy Bands in Crystals of Wurtzite Type'. Part I discussed the 'Symmetry of Bands Disregarding Spin-Orbit Interaction' [7]. In the second part with the subtitle 'Symmetry of Bands with Spin-Orbit Interaction Included' [8] published with Sheka, the authors demonstrated that the spin splitting of the dispersion $E(\boldsymbol{k})$ of s electrons near the Γ point $\boldsymbol{k} = 0$ is linear in $\boldsymbol{k}$ and isotropic for $\boldsymbol{k}$ perpendicular to the wurtzite c axis so that we get a ring of extrema in the dispersion $E(\boldsymbol{k})$. It is this feature which we associate nowadays with Rashba SO coupling. However, Rashba's second paper appeared in a special issue of Fizika Tverdogo Tela that was not translated into English and that was hardly available even in the Soviet Union. Thus it became rather difficult to trace back the Rashba effect to its origin.

Indeed, this paper contains a much more comprehensive study than just the proper derivation of what we call today the Rashba effect, a fact which makes this work highly interesting for current research on materials

with unusual dispersion curves. For this reason, we have appended an English translation[1] of this 'hidden jewel' which we hope will stimulate current research activities. Similar to Dresselhaus' work [5], Rashba and Sheka [7, 8] considered not only the Γ point $\boldsymbol{k} = 0$, but all symmetry points in the Brillouin zone. This was due to the fact that in 1959 the location of the valence and conduction band edges in $\boldsymbol{k}$ space was not yet firmly established for many semiconductors. More complete band structure calculations for zincblende and wurtzite semiconductors appeared much later [9, 10].

Related work was done by several authors including Glasser [11], Casella [12, 13], and Balkanski and des Cloizeau [14]. Yet two features set Rashba's early work apart from these other studies. Firstly, it was more comprehensive. In particular, it included an explicit model for the k-linear spin splitting. Secondly and more importantly, Rashba's work from 1959 was not just in hindsight a breakthrough, but it was the starting point for a visionary sequence of studies on SO coupling effects in solids. In a series of papers, Rashba and coauthors studied the remarkable observable consequences of the k-linear SO coupling in wurtzite materials [15–18]. In particular, the coupling between the configurational and spin motions makes it impossible to separate the quantum transitions in a magnetic field into purely configurational and purely spin ones [19], an effect Rashba coined 'combined resonances' [15]. The transitions thus provide a unique fingerprint for the nature of SO coupling. While this work was initially motivated by the k-linear SO coupling in wurtzite materials, Rashba *et al* expanded their analysis to zincblende materials [20–22] that were becoming increasingly popular at that time. This seminal theoretical work was done with little experimental motivation. It anticipated many concepts and ideas that have formed the foundations of today's spintronics, see Rashba's review [19]. Another early review of this field was given by Yafet [23] that covered also a range of related topics. Experimental verifications of the predicted phenomena followed only later [24–26]. A more complete review of combined resonances (also called electric dipole spin resonances) can be found in [27]. This early work focused solely on bulk semiconductors. Remarkably, we have lately observed a renaissance of the 'bulk' Rashba effect with the discovery of strong SO effects in layered bulk materials like BiTeI [28, 29], which is discussed in more detail below.

In the 1970s, quasi two-dimensional (2D) semiconductor systems became increasingly popular. Spin splitting in such systems was studied first by Ohkawa and Uemura [30] who considered the quantized states in the inversion layer on the surface of narrow-gap semiconductors. This theoretical work predicted a large k-linear term in the 2D dispersion relation due to SO coupling. It was inspired by experiments by Antcliffe *et al* [31] showing a beating pattern in the Shubnikov-de Haas oscillations measured for n-type inversion layers on $Hg_{0.79}Cd_{0.21}Te$ samples. Often, such beating patterns are taken as an indication for a spin splitting in the 2D dispersion. Yet in the particular case of Antcliffe *et al* [31], the beating was likely due to the occupation of multiple electric subbands [30].

Subsequently, Vas'ko and Prima [32, 33] studied theoretically the consequences of the k-linear splitting in quasi-2D systems, including combined resonances and the non-equilibrium spin polarization induced by a lateral electric field, nowadays often called the Edelstein effect [34]. In the 1970s, only few experiments [35] motivated such studies.

In 1984 Bychkov and Rashba [36, 37] pointed out the analogies between the k-linear spin splitting in bulk wurtzite and spin splitting in quasi-2D systems, which implies that many findings derived previously by Rashba *et al* for bulk wurtzite materials are likewise relevant for quasi-2D systems. This theoretical work was inspired by earlier experiments by Stein *et al* [38] and Störmer *et al* [39]. Stein *et al* [38] studied electron spin resonance on GaAs-$Al_xGa_{1-x}As$ heterostructures at finite magnetic fields B, suggesting a nonzero spin splitting even in the limit $B \to 0$ [40]. Störmer *et al* studied magnetotransport in a 2D hole system where they observed two distinct sets of Shubnikov-de Haas oscillations suggesting a spin splitting of the hole states [41, 42].

The spin splitting in a bulk zincblende or wurtzite semiconductor is an intrinsic property that cannot be altered in a given material. In quasi-2D systems the magnitude of the Rashba SO coupling depends on the shape of the effective potential seen by the charge carriers which can be tuned by means of external electric gates. In 1990, Datta and Das [43] proposed the famous spin transistor where the electron spins precess in the effective magnetic field due to SO coupling. By tuning the SO coupling via gates one can thus control the flow of electron spins between spin polarized (ferromagnetic) source and drain contacts. The tunability of Rashba SO coupling in quasi-2D semiconductor structures was first verified experimentally by Schultz *et al* [44], Engels *et al* [45] and Nitta *et al* [46]. This tunability has much inspired the research field of spintronics. Subsequent work has studied a wide range of phenomena related to the tunable Rashba SO coupling and it has remained a very fruitful area of research until today.

The Rashba effect has ever been influencing new material classes, the most important being the extension from semiconductors [47] to surfaces of metals [48]. The first observation in angle-resolved photoemission spectroscopy (ARPES) from metal surfaces succeeded in 1996 on the Au(111) surface [49], where the authors already pointed out the importance of both the surface gradient and the steep nuclear Coulomb potential in

[1] English translation available as supplementary material at stacks.iop.org/NJP/17/050202/mmedia.

heavy elements that made the observation possible. This has been directly confirmed by comparing Li-covered (110) surfaces of W and Mo [50] and the role of both contributions have been clarified theoretically by tight-binding models [51] and density-functional theory (DFT) calculations [52]. The Rashba splitting of Au(111) became widely known through high-resolution photoemission work [53]. An important confirmation of the Rashba splitting was obtained through direct measurement of the spin texture by spin-resolved photoemission, first for a surface state on H-covered W(110) [54] and subsequently for Au(111) [55].

For Bi surfaces very large Rashba-type SO effects have been observed not only with ARPES [56], but also in scanning tunneling microscopy (STM) exploiting the 'spin-momentum locking' of the electrons and comparing the expected interference patterns for spinless and spinful cases [57]. The combination of Rashba effect and exchange interaction makes it possible to observe in ARPES even very small band splittings as demonstrated for clean and oxidized Gd surfaces [58]. The above-mentioned spin-momentum locking plays an important role in the field of topological insulators [59]. Furthermore, it was observed that due to contamination of the surface by residual gases a band bending occurs at the Bi_2Se_3 surface, leading to the formation of a two-dimensional electron gas (2DEG); the strong SO coupling effects in this compound give rise to an increasing Rashba splitting of the 2DEG with increasing confining potential strength [60].

The largest Rashba-type SO effect so far has been found for a surface alloy of Bi/Ag(111) [61] where a Rashba coefficient $\alpha_R \approx 3.05$ eVÅ was obtained, while elemental surfaces such as Ir(111) can show values of α_R up to 1.3 eVÅ[62]. The idea of a Bi surface alloy has subsequently been transferred from a metal substrate to a semiconductor substrate, Si [63]. Si has also been used to study the Rashba effect of one-dimensional atom chains of Au [64] and for a Tl-induced surface structure [65]. Heavy elements can induce strong SO coupling effects in even the lightest elements, e.g., a large SO effect has been observed in the graphene Dirac cone by proximity to Au [66].

At this point we should note that the concept of Rashba effect is applied here to states that can be rather different from the 2DEG discussed by Bychkov and Rashba [36, 37]. In the field of semiconductors it was realized early that hole states, which carry not only spin but also orbital angular momentum, show an intricate behaviour both in spin splitting and spin polarization [67] that goes beyond the usual picture of the Rashba effect. Similarly, surface alloys, as the ones mentioned above, can exhibit spin splittings non-linear in $\boldsymbol{k}_{\parallel}$ and changes of the spin polarization within a single band [68].

More relevant for applications, investigations have recently shifted from surface effects towards interfaces and bulk. Rashba-split quantum well states (QWSs) have been reported in Au/W(110) and Ag/W(110) [69] and Pb/Si(111) [70]. As mentioned above, recently the Rashba effect was studied with renewed interest in bulk materials such as BiTeI [28, 29]. A Rashba effect was observed in several experiments [28, 71–73]. The observation of the relevant Rashba-split bulk states succeeded in ARPES [71, 72] and by Shubnikov-de Haas measurements [73].

Research has also been expanded to new compounds such as heterostructures combining the Rashba effect in semiconductors with superconductors, motivated in part by the search for Majorana fermions [74]. Another system of interest are oxide heterostructures that are insulating in the bulk but superconducting at the interface. Here it is suspected that the Rashba-type SO coupling at the interface may play an important role in the formation of the superconducting state [75].

The present focus issue gives an overview of current research on Rashba physics ranging from semiconductors to ultracold atoms. In semiconductors it is not straightforward to discriminate experimentally between the relative contributions of Rashba and Dresselhaus SO coupling. Here Wilde and Grundler [76] demonstrate theoretically for 2D systems that magneto-oscillations in a tilted magnetic field provide a new pathway to achieve this goal. Several related studies focus on how Dyakonov-Perel spin relaxation is influenced by the interplay of Dresselhaus and Rashba effective magnetic fields [77–79]. The Dresselhaus term depends strongly on the crystalline growth direction. Wang *et al* [77] have investigated symmetric and δ-doped asymmetric GaAs/AlGaAs (110) quantum wells, where Rashba and Dresselhaus effective fields are perpendicular to each other. This leads to an anomalous dependence of the spin relaxation on an external magnetic field [77]. For GaAs/AlGaAs (111) quantum wells, Balocchi *et al* [78] demonstrate experimentally that the spin relaxation anisotropy can be either canceled or inverted by an electric bias. This effect is quantitatively described in the framework of a spin density matrix formalism.

Golub and Ivchenko [79] have developed a general theory of current-induced spin orientation in 2D semiconductor systems for the streaming regime of transport, where the electrons accelerate ballistically until they reach the energy of optical phonons. The Dyakonov-Perel spin relaxation is drastically modified in this regime. The current-induced spin orientation increases from ~0.1% in weak fields to ~2% for $E \sim 1\,\mathrm{kV\,cm^{-1}}$ due to the anisotropic momentum distribution and decreases again when the field is increased further. Moreover, field-induced oscillations of the spin polarization of photocarriers are predicted for particular fields in this regime [79]. Spin filters based on a single loop are promising as spin valves or analyzers. Matityahu *et al* [80] demonstrate theoretically that an interferometer made of two quantum dots or quantum nanowires with

strong SO interaction and threaded by an Aharonov-Bohm flux can serve as a perfect spin filter. Under this condition, perfect symmetry between the two branches is not required.

For silicene, Geissler *et al* [81] derive a model Hamiltonian from a group theoretical analysis including the Rashba SO interaction. While in graphene the intrinsic SO interaction has to be larger than the Rashba SO interaction to obtain the quantum spin Hall phase [82], the situation is different for buckled silicene, where the sublattice symmetry is broken. The authors show that the quantum spin Hall insulator phase can be generated in silicene by Rashba SO interaction [81].

In metal-covered semiconductors a breaking of the spatial inversion symmetry occurs both for the QWSs of the metal and for the electrons in the space-charge region of the semiconductor. The latter is observed directly by Lin *et al* [83] with ARPES for Ge(111) covered by two layers of Pb. Most states in the space-charge layer can be derived from the bulk band edges of the semiconductor, but additionally—as a direct consequence of the Rashba effect occurring at the interface to the metal—these experiments show the appearance of a 'non-split-off' band derived from strongly SO-split states. The spin splitting of the QWSs of Pb films on Si(111) is likewise an effect of SO coupling in an inversion asymmetric environment that can be observed in spin-resolved ARPES measurements [70]. Slomski *et al* [84] observe a hybridization between such Rashba-split bands of opposite spin polarization, indicating that interband SO coupling is important in the interaction of these QWSs. DFT calculations and spin-resolved ARPES experiments demonstrate this spin-mixing effect mediated by SO coupling in Pb films on Si.

The 3D Rashba splitting and Rashba-split surface states have been studied by Landolt *et al* [85] for BiTeCl, and Eremeev *et al* [86] for BiTeBr and BiTeI. ARPES and structural investigations show that the surface electronic structure of BiTeI depends sensitively on the termination and extrinsic and intrinsic defects. Fiedler *et al* [87] point out that bulk stacking faults that invert the order of the stacking sequence can lead to two coexisting domains with different surface terminations. DFT calculations show that the Te-terminated surface of BiTeBr gives rise to a giant Rashba parameter of $\alpha_R \sim 2$ eVÅ [86]. BiTeCl is also identified as a 3D Rashba system with a large bulk band gap [85]. A large Rashba splitting of the bulk band is observed by ARPES and DFT. The Te termination shows Rashba-split surface states; the Cl termination, however, undergoes photon-induced changes of stoichiometry [85]. Also, on the topological insulator Bi_2Te_2Se with a composition tuned to the topological transport regime, Miyamoto *et al* [88] observe a surface state with giant Rashba splitting in the occupied states by spin-resolved ARPES. The authors point out that the magnitude of the splitting is compatible with requirements for nanoscale spintronic devices.

Au(111) and W(110) have emerged as model systems for Rashba effects at metal surfaces [49, 50, 53–55]. While previously the occupied part of the Rashba-split Au(111) surface state was the focus of investigation [49, 53, 55], Wissing *et al* [89] now investigate also the unoccupied part by spin- and angle-resolved inverse photoemission, tracing it up to the band gap boundary. Moreover, they observe a spin dependence of bulk transitions. Using one-step model calculations of the inverse photoemission process, they explain their observation as initial-state effects.

The W(110) surface gives rise to Dirac-type surface states establishing a connection between Rashba and topological insulator physics. This feature has partially been observed before [54] and has been studied more recently with spin resolution [90, 91]. The circular dichroism obtained in ARPES due to this surface state is analyzed using DFT coupled to one-step photoemission calculations taking into account initial and final states [92, 93], Calculations of spin-dependent two-electron emission from this state by Mirhosseini *et al* [92] show that measurements of the spin dependence of the exchange-correlation hole become feasible. Braun *et al* [93] interpret the linear dispersion of W(110) surface states as the result of a very sensitive interplay between SO interaction, relaxation of the first atomic layer and enhanced charge transfer at the surface. They obtain almost quantitative agreement between photoemission calculations and experiment at low photon energies, and they predict that the Dirac-like surface states give rise to unusual features that may even be observed using hard-x-ray photoemission at 30 keV [93].

The modification of the spin-dependent surface electronic structure of W(110) by monolayer adsorbates turns out to be rather complex. Shikin *et al* [94] compare Au, Ag and Cu monolayers by spin-resolved ARPES and DFT calculations. In particular, they discuss why Ag/W(110) shows a larger Rashba SO splitting than Au/W (110) despite the smaller atomic number. The influence of the strong SO interaction in W(110) extends also to QWSs, e.g., in Au and Ag overlayers. By comparison between a W(110) substrate and Mo(110) as a control sample, Shikin *et al* [95] find that QWSs of *sp* type are much more affected than those of *d* type due to different degrees of localization.

Atomic and interfacial potential gradients affect the Rashba splitting in complex ways, as is revealed by several studies on very different metal systems [94–96]. The giant Rashba splitting of the Ir(111) surface state with $\alpha_R \sim 1.3$ eVÅ exists also underneath a graphene overlayer, but the surface state does not intersect the Fermi energy. Using spin-resolved ARPES, Sánchez-Barriga *et al* [96] show that this state can be moved upwards and downwards in energy without affecting the Rashba splitting by increasing the number of graphene layers and

decorating them with Ir, Au, and Fe clusters, respectively. The results are supported by DFT calculations including Green function embedding for a semi-infinite geometry.

Takayama *et al* [97] use thin films of Sb(111) and Bi(111) on Si to study the Rashba-split surface states by spin-resolved ARPES: a reduction of the spin polarization away from the surface Brillouin zone center is observed for Sb which does not appear for Bi and indicates strong interaction with bulk states. Ultrathin Bi films on an insulating substrate permit an investigation of transport effects of the Rashba-split Bi(111) surface states. Using a four-tip STM, Tono *et al* [98] measure transport for tip-tip distances below 1 μm. A magnetic CoFe-coated carbon nanotube tip in comparison with a Pt-coated tip allows to detect current-induced spin polarization due to the surface state. A quantitative theoretical analysis supports this result.

A Rashba-type SO splitting occurs also in atomic chains [64]. Crepaldi *et al* [99] study chain-like surface alloys of Bi and Pb on Cu(110) using ARPES and DFT. The interaction with bulk Cu states leads to open and warped Fermi surfaces and a k-dependent spin splitting perpendicular to the chains. The authors also find that the splitting in $Bi_{1-x}Pb_x$ overlayers can be tuned by changing the stoichiometry. Surface alloys of Bi/Ag(111), Cu/Ag(111), and Pb/Ag(111) display giant Rashba splittings of occupied and unoccupied states, respectively. El-Kareh *et al* [100] study the quasiparticle interference for Pb/Ag(111) using STM and compare to the theoretically predicted spin polarization. The inertness of the Bi/Ag(111) surface alloy permits Cottin *et al* [101] to grow organic molecules which interact very weakly with the substrate so that the surface state is also unaffected. Using ARPES, Bentmann and Reinert [102] show that Na deposition enhances the Rashba splitting of the Bi/Cu(111) surface alloy whereas it is reduced by Xe. This result is explained based on the spatial distribution of the wave functions.

Significant experimental advances, as have been witnessed in spintronics and ultracold atomic gases, often permit a new view on fundamental concepts that so far had little or no chance to be realized experimentally. The concept of generalized spin electromagnetic fields is very useful in spintronics where, e.g., a spin electric field generates a spin current and a spin magnetic field drives a spin Hall effect. Nakabayashi and Tatara [103] extend the expressions for generalized spin electromagnetic fields under strong s-d exchange interaction for the Rashba interaction. Among other results, extremely high electric and magnetic fields are predicted for nanoscale structures. Experimental advances in SO-coupled cold atoms and topological insulators constitute also the motivation to investigate how SO coupling influences the quantum mechanical measurement process. Sherman and Sokolovski [104] consider a von Neumann or projective measurement of spin: in one example, spin dynamics are mapped on a spatial walk, and the measurement-time averages of the spin components σ_x and σ_y can be measured in a single short-time measurement. Fialko *et al* [105] consider a prototypical quantum spin Hall system analytically and numerically: consequences for realizing a fractional quantum spin Hall effect in electronic or ultracold atom systems are pointed out. When a normal metallic state is subjected to a Zeeman field, the different Fermi surfaces for spin-up and -down electrons can lead to superconducting pairing with the two Fermi surfaces displaced. This anisotropic superfluid phase is known as Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase and being sought for in Fermi gases of ultracold atoms. Dong *et al* [106] study a fermionic cold atom system subjected to a Zeeman field and additionally to three-dimensional isotropic SO interaction. An FFLO phase with asymmetric momentum distribution robust against interaction and finite temperature is obtained.

In closing, we hope that the quality and diversity of the results presented in this Focus Issue demonstrate that more than 50 years after its discovery the Rashba effect continues to be a source of inspiration for physicists that stimulates exciting and important new research.

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