FINAL REPORT

1 General Information

DFG reference number: BE 2464/21-1

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Project title: **Optimization of different strategies for designing an energy harvester based on spin-torque diodes**

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2 Summary

Summary in German: Die stetig wachsende Nachfrage nach billiger und grüner Energie hat eine rasche Entwicklung von so genannten "Energy Harvesting"-Geräten zur Erzeugung von Gleichstrom aus der in der Umgebung fast immer vorhandenen Mikrowellenstrahlung aus den Quellen wie Fernseh- und Mobilfunknetzen, Wi-Fi-Routern usw. ausgelöst. Die Energiedichte dieser Strahlung reicht von 1 bis 1000 nW/cm^2, so dass die entsprechende Technologie erfolgreich für Anwendungen mit geringer Leistung vorgesehen ist (Digitalthermometer, Rauchmelder, einige Sensortypen in der Medizin usw.). Das Hauptziel dieses Projekts war die Optimierung verschiedener Designs für solche ‚Energy Harvester' auf der Basis von Spin-Torque-Dioden - Geräten, bei denen Gleichspannung erzeugt wird, wenn ein Wechselstrom durch einen magnetischen Tunnelübergang (MTJ) fließt. Mit Hilfe von Computersimulationen haben wir folgende drei Haupttypen von MTJ-basierten Nanosystemen untersucht und Wege für deren Optimierung vorgeschlagen: (i) "Standard"-MTJ-Nanosäulen mit der fast homogenen Magnetisierungsoszillationen in der Schichtebene; (ii) MTJs im Präzessionsregime senkrecht zur Schichtebene (für die Breitbandrektifikation) und (iii) Schichte mit der speziellen Form, wo Oszillationen der Domänenwände (DWs) auftreten. Wir haben u.a. optimale geometrische und magnetische Parameter und die maximale Effizienz der Rektifikation für alle diese Arten von Energie-Harvestern vorhergesagt.

Summary in English: Steadily growing demand for cheap and green energy has caused a rapid development of so called 'energy harvesting' devices for producing dc-power from the ambient microwave radiation from various sources like TV and mobile-phone networks, Wi-Fi routers etc. The energy density of this radiation ranges from 1 to 1000 nW/cm^2, so that corresponding technology could be successfully used by low-power applications (digital thermometer, smoke detectors, some sensors in medicine etc.). The main goal of this project was the optimization

of various designs for energy harvesters based on spin-torque-diodes (STDs), i.e. devices where dc-voltage is generated when an ac-current flows through a magnetic tunnel junction (MTJ). Using computer simulations, we have studied and optimized three main types of MTJ-based nanodevices: (i) ‘standard’ MTJ nanopillars of the resonant type employing quasi-homogeneous in-plane magnetization oscillations; (ii) MTJs in the out-of-plane precession regime for broadband rectification and (iii) multilayer stacks with the in-plane shape designed for oscillation of domains walls. As the results of this project we have determined optimal geometric and magnetic parameters for all three kinds of spin-torque-based energy harvesters listed above, and predicted corresponding maximal rectification efficiencies in ambient conditions.

3 Progress Report

3.1 Background and objectives of the project

Project background: Design of optimal energy harvesters based on STDs is still under development. Computer-aided optimization of these systems by full-scale micromagnetic simulations and taking into account thermal fluctuations would greatly improve our physical understanding of rectification processes in MTJ stacks and thus allow to predict optimal device features for energy harvesting. The background of the GNRL group led by Dr. D. Berkov (see publications cited in the project application), clearly demonstrated the efficiency of our numerical methods for simulations of magnetization dynamics, including the non-linear dynamics induced by spin torque. Hence we had all the necessary competence for the development of new methods and concepts required for the prediction of the efficiency of STD-based energy harvesters and their optimization, which is required for the achievement of project goals.

Objectives of the project: The main project goal was the numerical optimization of various types of energy harvesting nanodevices which employ the STD effect and the prediction of the best possible performance of STDs intended for the energy harvesting. For this purpose, three main types of nanodevices based on magnetic tunnel junctions were investigated:

(i) Resonant-type STDs based on MTJs nanopillars with in-plane magnetization oscillations;

(ii) Broadband STDs employing MTJs with the perpendicular magnetic anisotropy (PMA), where the out-of-plane precession regime was expected;

(iii) Multilayer stacks of nanostripes with the specially designed in-plane shape allowing the existence and oscillation of domains walls (DWs).

3.2 Description of the project-specific results and findings

Work package 1 (WP1): Optimization of a single resonant-type in-plane-precession MTJ

1. We have suggested two new methods of micromagnetic simulations for the calculation of the STD-rectified voltage V_{dc}; both of them allow to compute the whole frequency dependence $V_{dc}(f)$ in a single simulation run. The first method uses the input current which is a discrete sum of *N* harmonic signals and accelerates simulations by the factor of *N*. The second method employs a ‘sinc’ current pulse with a continuous power spectrum. This approach provides a very high spectral resolution limited only by the length of the sinc-pulse and leads to the correspondingly large acceleration degree. For this reason the sinc-pulse is clearly the method of choice by simulations at $T = 0$. For $T > 0$ the method using the sum of harmonic signals may be faster (although the resolution is lower), due a better signal-to-noise ratio, which enables a faster accumulation of the required statistics.

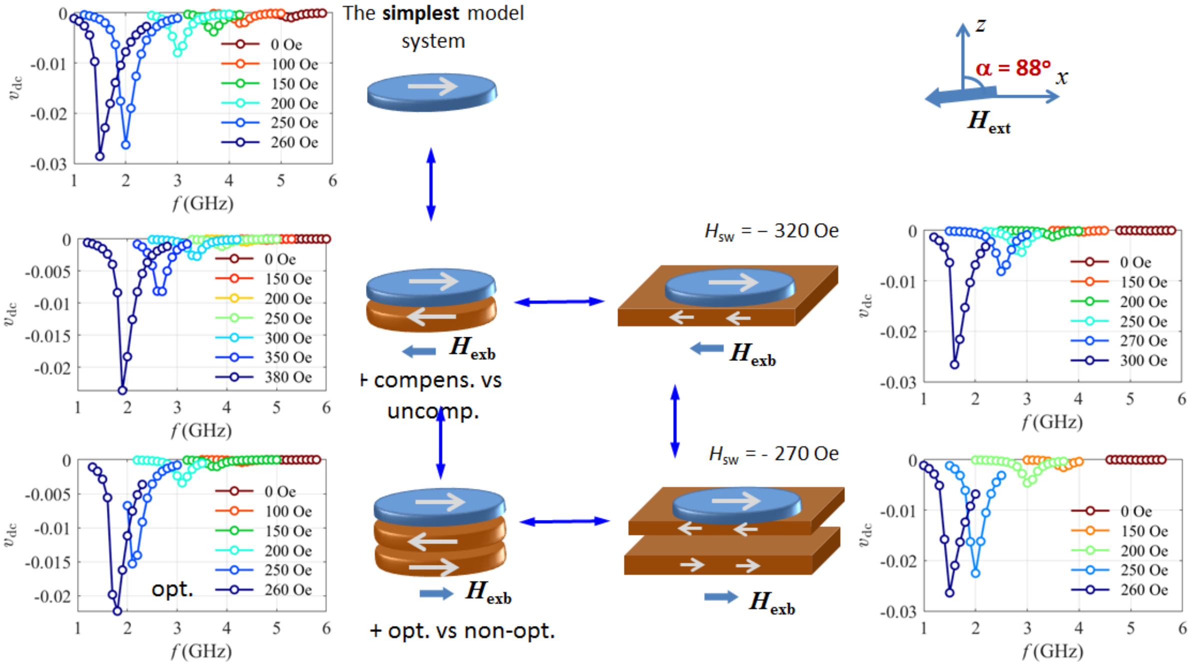

Fig. 1.1 Cumulative picture of five different designs for an ‘in-plane’ STD usable as an energy harvester together with corresponding dependencies $V_{dc}(f)$ at different external fields. See text for more details.

2. We have studied four possible designs of a MTJ stack which be used as an energy harvester: (i) double layer stack with both free and fixed layers being patterned, (ii) three layer stack (free layer + AAF) with all layers patterned, (iii) double-layer stack with the unpatterned fixed layer and (iv) three layer stack with the unpatterned AAF. Cumulative results (together with the free layer only) taken as the reference system are shown in Fig. 1.1 as frequency dependencies of the rectified voltage for various applied fields (less than the switching field of the free layer for each system). Interestingly, the maximal obtained reduced dc-voltage $v_{dc} = V_{dc}/(I_0 R_0)$ (I_0 is the amplitude of the ac-current, R_0 – the zero-current resistance of the MTJ stack) depends very weakly on the studied design and is only slightly smaller than for the single-layer system, where no magnetization oscillation energy can be transferred to other stack layers. Detailed analysis of these results is postponed to the future publication.

3. We have investigated the fundamental efficiency limit of an ’in-plane’ STD, analysing the dependence of the maximal V_{dc} on the external field H_{ext}. We have shown that this maximal value rapidly increases when H_{ext} approaches the switching field H_{sw} of the STD free layer due to the increase of dc- and ac-susceptibilities of the system, so that the difference H_{sw} - H_{ext} should be made as small as possible. However, it should be large enough to ensure a sufficiently high energy barrier between the metastable state used for the dc-voltage generation (on the upper branch of the hysteresis loop) and the energetically more favourable equilibrium state on the lower loop branch. Here we have demonstrated that this energy barrier in presence of an ac-current is nearly the same as without any current, in contrast to the case of the dc-current. Using this feature, we could predict the field value where V_{dc} is much larger than for $H_{ext} = 0$, whereby this field is still far enough from H_{sw}, so that the thermal stability is ensured. Detailed results can be found in our paper [1] (see attachment). Our findings can be used by optimizing energy harvesters based on standard ’in-plane’ nanoelements and to predict the maximal voltage which could be achieved for this STD type.

WP2: Development of an array of resonant-type STDs to obtain a broadband rectifier

In this WP we have proposed and theoretically elaborated a new approach for constructing broadband ac-current rectifiers from resonant-type in-plane STDs. Their intrinsic bandwidth, being constrained by the FMR linewidth of the corresponding MTJ, is relatively narrow, what is a significant limitation. To address this issue, we have proposed to use an array of these STDs, each with a distinct resonance frequency. By ensuring that the frequency difference between adjacent STDs is smaller than their individual bandwidths, we could construct a device capable of rectifying signals over an almost arbitrarily broad frequency range. To verify the effectiveness of our approach, we have performed analytical calculations, macrospin modelling and full-scale micromagnetic simulations.

Our analytical calculations have shown that, although the resonant frequency of an elliptical nanoelement obviously depends on its shape (via the demagnetizing coefficients), the maximal value of the rectified voltage is nearly shape-independent. This feature is very favourable for the construction of the broadband rectifier.

From the methodical point of view we have shown that the macrospin approach provides qualitatively correct results, but for the quantitative description of the magnetization dynamics and the resulting dc-voltage the usage of full-scale micromagnetic simulations is mandatory even for nanoelements as small as studied in this WP (e.g., 100 x 200 nm^2). This is especially true when thermal fluctuations are present, as it is the case in any real application. The reason is, that micromagnetic simulations capture the local variations of thermal noise and magnetization, which are not accessible in the macrospin approximation.

Our physical results show that the performance of STD arrays in producing the rectified voltage can be nearly frequency-independent in a range much broader than the resonance line width of their individual elements, thus making them to promising candidates for the broadband energy harvesting. Corresponding analytical and numerical results are described in detail in our paper [2]. Our research establishes the groundwork for the development of broadband energy harvesters based on arrays of resonant-type STDs, with potential applications in various fields requiring efficient energy conversion across a wide frequency spectrum.

After our theoretical study was finished, we have learned about the independent experimental implementation of the same idea in the paper of Sharma et al. (*Nature Electronics*, **7** (2024) 653), which support our results and addresses the technical problem discussed above.

WP3: Prediction of the optimal design for *out-of-plane precession* devices taking into account regular and quasi-chaotic precession regimes

Instead of optimizing only the out-of-plane precession regime of STDs - as stated in the title of this work package – we have studied the complete transition between the in-plane and out-of-plane precession regimes, because it has turned out that the system demonstrates the most interesting and promising behaviour in course of this transition.

We have performed corresponding simulations both for the macrospin approximation and in the full-scale micromagnetic approach. Due to the lack of space, we present here only macrospin results, micromagnetic results can be found in the attached presentation.

As in WP2, we have simulated the system consisting of the free MTJ layer only (Fig. 3.1(a)). For the macrospin approach, the shape anisotropy of the nanoelement was taken into account via demagnetizing coefficients, and the out-of-plane anisotropy energy contained both the first- and second-order terms. We have set the element magnetization to $M = 1000$ G, and the ratio between the anisotropy constants to $K_2/K_1 = 0.03$. Keeping in mind that for the energy harvesting applications only a relatively small signal power is of interest, we have used the ac-current density amplitudes $J_0 = 1 \times 10^9 \ldots 1 \times 10^{10}$ A/m^2. The transition between the in-plane ($\theta = \pi/2$) and out-of-plane ($\theta = 0$) equilibrium states by increasing the perpendicular anisotropy constant occurs around the value $K_1 = 5.7 \times 10^6$ erg/cm^3 (see Fig. 3.1(b)).

Magnetization dynamics of the obtained system is highly non-trivial, what can be seen already from the anisotropy dependence of the resonant frequency $f_{res}(K_1)$ in Fig. 3(c). The two minima in this dependence correspond to K_1 values at transitions points between purely in-plane/out-of-plane states and the interval of intermediate moment orientations ($0 < \theta < \pi/2$). At such points, where a ‘pure’ precession regime (‘in-plane’ or ‘out-of-plane’) changes to a ‘mixed’ one, the energy landscape becomes nearly flat, what leads to the strong decrease of the oscillation’s eigenfrequency.

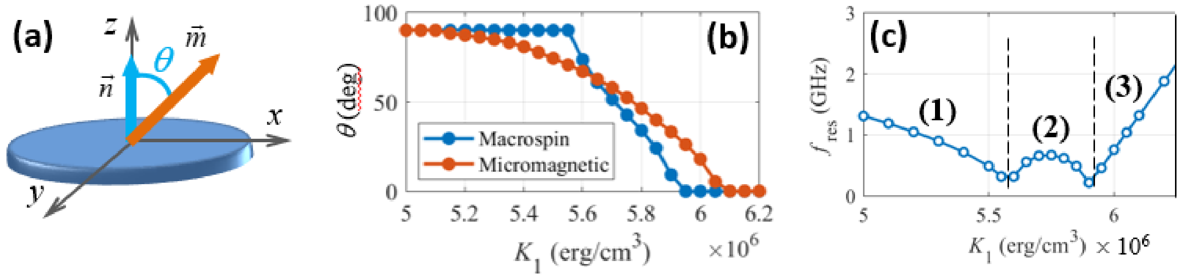

Fig. 3.1 (a) Simulated system, (b) dependence of the equilibrium magnetization angle on the first anisotropy constant K_1 in the macrospin approximation and from micromagnetic simulations, (c) dependence of the resonance frequency on K_1 for the macrospin at T = 0 K with the marked anisotropy intervals (1), (2) and (3) to be used in Fig. 3.2.

Frequency dependencies of the dc-voltage at three K_1 intervals marked in Fig. 3.1(c) as (1) (2) and (3), are shown in Fig. 3.2. The plots $v_{\rm dc}(f)$ in the panel (2) are shifted by δv = 0.01 for the better visibility, because the dependence $f_{\rm res}(K_1)$ for the interval (2) is not monotonic.

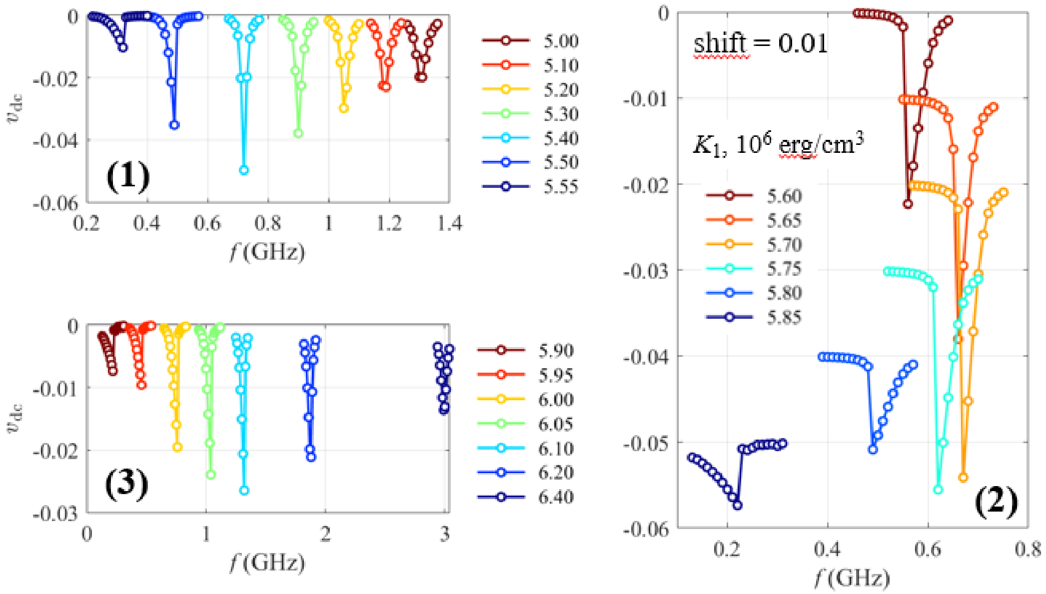

Fig. 3.2 Frequency dependencies of the rectified voltage at T = 0 K for all first anisotropy constants K_1 studied in simulations. For better visibility, results for anisotropy intervals (1), (2) and (3) marked in Fig. 3.1(c) are shown in separate panels. For this example $J_0 = 2 \times 10^9$ A/m^2.

The same simulations have been performed for the ambient temperature T = 300 K. The main difference to the case of T = 0 K is the much larger width of the resonant lines $v_{\rm dc}(f)$ compared to those shown in Fig. 3.2. Anisotropy dependencies of resonant frequencies $f_{\rm res}(K_1)$ at T = 300 K are presented in Fig. 3.3(a) for all studied ac-currents amplitudes J_0 as shown in the legend. For the given anisotropy this frequency depends on J_0 relatively weakly (except the points near the minima of $f_{\mathrm{res}}(K_1)$), what means that magnetization oscillations at all studied currents are approximately linear almost for all values of K_1.

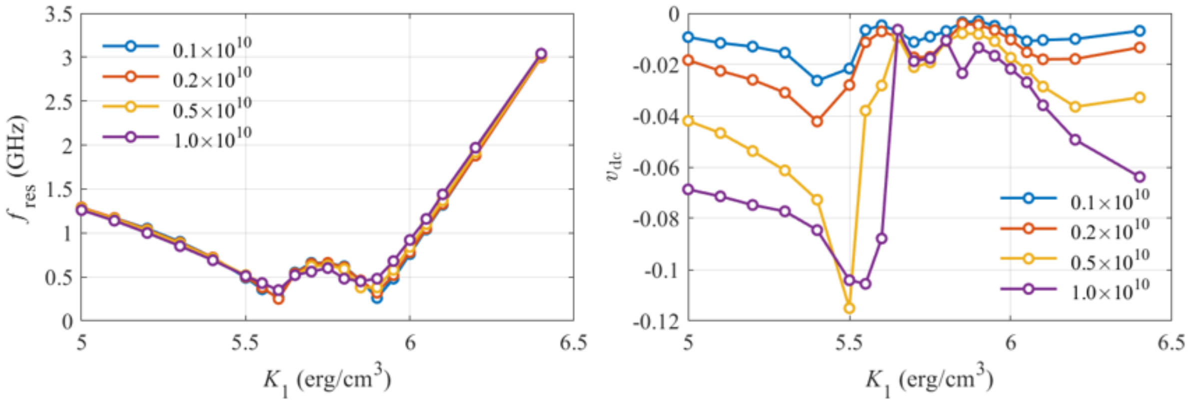

Fig. 3.3 Left panel: dependence of the resonance frequency on K_1 for the macrospin at T = 300 K. Right panel: dependence of the maximal rectified voltage on K_1 for the same system.

Finally, anisotropy dependencies of the maximal value of the rectified current $v_{\mathrm{dc}}(K_1)$ at T = 300 K are shown in Fig. 3.3(b). For all currents, the largest values of v_{dc} are observed in the anisotropy interval around $K_1 = 5.5 \times 10^6$ erg/cm^3, which corresponds to the 'transition' from the in-plane moment orientation to the tilted one. This means that these anisotropy values are the most favourable ones for constructing an energy harvesting STD for this geometry.

Due to the lack of space, further results of this WP for the macrospin approximation and for full-scale micromagnetic simulations are attached as the ppt-presentation for WP3.

We also note that quasichaotic precession regime was not observed for ac-current amplitudes which can be relevant for the energy harvesting applications.

WP4: Studies of the ac-current rectification due to DW oscillations in MTJ nanostripes

Similar to WP3, in this WP we have studied ac-current rectification for all out-of-plane anisotropy values including those where this anisotropy dominates the demagnetizing filed of a thin stripe ($K_1 = (1 \div 4) \times 10^6$ erg/cm^3); simulations for both (0,1,0) and (0,0,1) spin current polarizations were performed for all K_1 values.

In the first part of this WP we have used the stripe with two small semi-circular notches. Corresponding equilibrium magnetization of the domain walls can be found in the attached presentations. Stripes with the lateral size 800 × 100 nm^2, thickness 2 nm and material parameters M = 1000 G and $A = 1 \times 10^{-6}$ erg/cm were simulated; current flow was localized in the central stripe region (Fig. 4.1, upper image on the left panel). When only the Slonczewski term was taken into account, the resulting dc-voltage was relatively small for all ac-current amplitudes (1×10^9 to 1×10^{10} A/m^2) relevant for the energy harvesting applications and in the entire interval of anisotropies (Fig. 4.1, left panel). Detailed studies have revealed that the reason for this relatively small output is the strong localization of magnetization oscillations near the notches (examples for several anisotropies are shown in Fig. 4.1, right panel), resulting in the decrease of the average amplitude of these oscillations within the current mask. An interesting feature of the generated *reduced* dc-voltage is the decrease of its maximal value in the current interval from 1×10^9 to 1×10^{10} A/m^2. The analysis has shown that this feature is due to the change of the phase shift between current and magnetization oscillations.

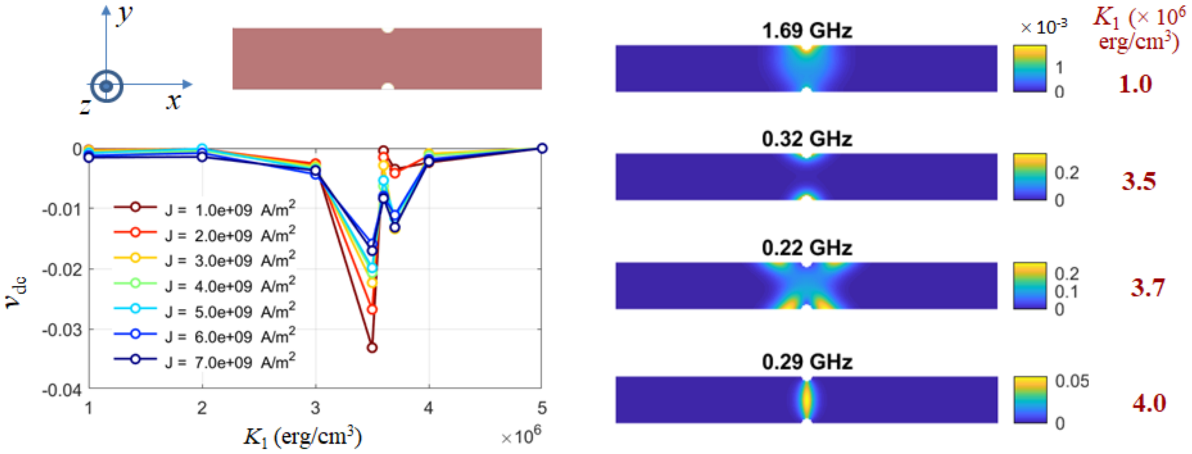

Fig. 4.1 Left panel from top to bottom: coordinate system and the stripe shape with two small semi-circular notches; dependence of the maximal rectified voltage on the anisotropy constant for ac-current amplitudes shown in the legend. Right panel: oscillation power maps for different perpendicular anisotropies. Spin polarization direction is **s** = (0,0,1).

In order to improve the harvesting efficiency, we have tried several other stripe shapes and included the field-like torque term into the LLG equation used in simulations. The relative factor c_{fl} for this term (with respect to the Slonczewski torque) can be quite large, achieving the value $c_{fl} = 0.4$ for some materials (see, e.g., Skirdkov et al, *Appl. Phys. Lett.* **113**, 242403 (2018)).

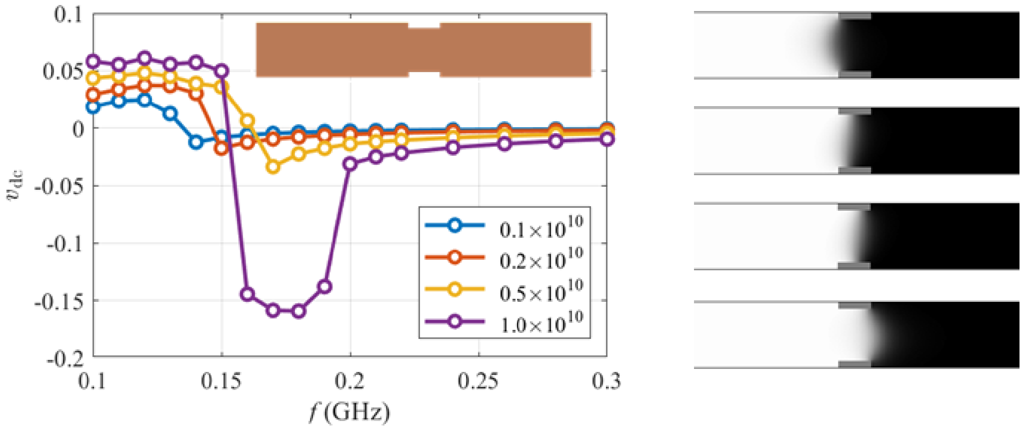

Fig. 4.2 Left panel: frequency dependence of the dc-voltage at ac-current amplitudes shown in the legend for out-of-plane domains (K_1 = 4 x 10^6 erg/cm^3) and the stripe shape with two rectangular notches (inset); Right panel: domain wall oscillations shown as four subsequent DW positions. Spin polarization direction is **s** = (0,0,1).

Among several simulated designs and combinations of the material parameters best results have been obtained for the stripe with two rectangular 50 × 10 nm^2 notches (Fig. 4.2, inset on the left panel). The flat shape of such an inset leads to an almost flat energy landscape for a domain wall created between the notches, so it can be shifted relatively easy between its limiting positions at the left and right ends of the notches (Fig. 4.2, right panel). These oscillations are also promoted by the field-like spin torque term, fully analogous to DW oscillations produced by the corresponding oscillated 'real' magnetic field. In the left panel of Fig. 4.2 it can be seen that the *reduced* dc-voltage produced by this design is about 5x larger than for the circular notches and the when only the Slonczewski term is included.

More results for this WP can be found in the attached presentation.

3.3 Deviations from the original concept; findings that contradict initial hypotheses

WP1: In contrast to initial expectations, we have found that the energy harvesting efficiency by in-plane resonant-type STDs designed as MTJ stacks, depends relatively weakly on the stack geometry (see Fig. 1.1). Although this result is negative with respect to the STD optimization, it is still important for the implementation of this harvesting technology, because it means that the MTJ stack design can be guided only by its reliability and implementation simplicity.

WP2: The independence of the maximum of the generated dc-voltage on the nanoelement's shape was unexpected; however, this feature has greatly assisted by the design of the broadband energy harvester (see [2]).

WP3: New data obtained during the project have required simulations of the harvesting efficiency not only for purely in-plane and perpendicular-to-plane precession regimes, but also for anisotropy values corresponding to the transitions between these two regimes. Maximal efficiency has been observed for anisotropy values at the beginning and end of this transition.

3.4 Activities and approaches to quality-enhancing measures through which the validity or verifiability of your research findings was ensured

All newly developed numerical methods where verified by analytical calculations (see, e.g., Sec. II of [2]) or at least by already well established – but much slower - numerical methods (see, e.g., Sec. II of [1]). In addition, we have constantly analyzed the experimental literature in order to find papers published after the project start, which would confirm or contradict our theoretical findings. In particular, the (independently conducted) experimental work of Sharma et al, *Nature Electronics*, **7** (2024) 653 has confirmed our results from WP2 [2].

3.5 Description of the handling of research data generated in the project and the data infrastructures used

All research data generated (using numerical simulations) in frames of this project are saved on data storage devices in corresponding workstations, with additional backups on external hard disks. There are no special legal obligations concerning the handling of our data. After all our results will be published, corresponding data will uploaded to the Material Cloud Archive (https://archive.materialscloud.org/) which at the moment seems to be the only suitable cloud for our data type. The project leader Dr. D. Berkov is responsible for the proper handling of the research data obtained within this project.

3.6 Description of any research data, methods and software generated in the project that are re-usable and openly accessible to others

As explained in the description of results in WP1, we have developed two new methods for the calculation of the STD-rectified voltage in a single run, which provide a very high acceleration of corresponding simulations. Both methods are described in detail in our paper [1] and thus are openly accessible. Further, all data used for producing the plots of our results in project-related papers will be made openly accessible in repositories listed in the previous subsection, after the corresponding papers are published in peer-reviewed journals.

4 Published Project Results

4.1 Publications with scientific quality assurance

[1] D. Berkov, E.K. Semenova, Numerical studies of the fundamental efficiency limit of a resonant in-plane spin-torque diode, *Phys. Rev. Applied*, **22**, 044040 (2024)

[2] E.K. Semenova and D. Berkov, Array of resonant-type spin-torque diodes as a broad-band rectifier: Numerical studies, *J. Appl. Phys.*, **136**, 083907 (2024); **(Editor’s pick)**

[3] D. Berkov, E. Semenova, Phase diagrams of precession regimes in spin-torque diodes for energy harvesting, Talk on the international conference *Trends in Magnetism 2023*, Rome, Italy, 4-8 Sept., 2023

[4] D. Berkov, E. Semenova, Performance analysis of the spin-torque-based energy harvester in the transition region between in-plane and out-of-plane precession regimes, Talk on the international conference *Trends in Magnetism 2025*, Torino, Italy, 25-28 May, 2025

4.2 Other publications and published results

[5] D. Berkov, E.K. Semenova, Prediction of the optimal design for the energy harvester based on the magnetization precession in nanoelements with the perpendicular magnetic anisotropy, Technical report, published on the Research Gate in the account of D. Berkov, url: https://www.researchgate.net/profile/D-Berkov

[6] D. Berkov, E.K. Semenova, Studies of the ac-current rectification arising due to DW oscillations in MTJ nanostripes, Technical report, published on the Research Gate in the account of D. Berkov (url see above)

In all publications from the list above the funding of the DFG is gratefully acknowledged.