Is There Chaos in Blobs of Carbon Nanotubes Used to Perform Computation?

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***Abstract*—We report on observations of the behavior in single-wall carbon nanotubes (SWCNTs) and polymer nanocomposites, which may indicate that the conductivity of this nanomaterial undergoes chaotic changes under certain circumstances. We present interesting material properties that can be used for (a) investigating non-linearity / chaotic behavioral properties of the material, (b) understanding the underlying physics that may be explored by evolution, and (c) identifying appropriate signal types (voltages, frequencies) suitable to stimulate the material and demonstrate a computationally rich behavior. The presented results show that the investigated material is particularly sensitive to specific frequencies, e.g., square waves, and suggest that different behavioral regimes may be achieved, e.g., uniform, stable, chaotic. This work is done within the NASCENCE project, whose goal is to find new materials suitable to perform computation.**

Keywords- Computation-in-Materio; Evolution-in-Materio; Evolvable Hardware; Chaos.

I. INTRODUCTION

Traditional silicon-based computers are meticulously designed with a conventional top-down process. The miniaturization and engineering of such processors poses technological and economical challenges. In contrast, Evolution-in-Materio [1] [2] is a bottom-up approach where the intrinsic underlying physics of materials is exploited as computational medium. Different computational substrates have been previously explored [3] [4] [5]. The EU-funded NASCENCE project [6] investigates how nano-scale materials, e.g., carbon nanotubes / polymer composites, liquid crystals, and graphene, may be used and configured to produce computation. As such, the material blob is treated as a black-box and is interfaced to a traditional computer through a series of signals / wires which send inputs / configurations and read / interpret outputs. Evolutionary algorithms are the means of finding suitable configurations in order to “program” the material to solve a wanted function. Such a black-box hybrid approach has been shown successful for different problems, such as Traveling Salesman [7], logic gates [8], bin packing [9], machine learning classification [10], frequency classification [11], and function optimization [12]. At the current state of research, it is not clearly understood what the exploited underlying physical properties are and what is the best way of exploring them, e.g., number of input / outputs, types of signals (static voltages, sinusoidal waves, square waves). The solved problems serve as proof of concept that such an approach may be competitive in terms of computational time, size, and energy consumption, but scaling-up to solve bigger instances requires a better understanding. In other words the black-box needs to be opened. The number of used input electrodes, configuration signals, etc., is related to what part of the search and solution space is available for evolution to be exploited on the material, which may be critical for the success of any kind of computational task.

There are several parameters that may have impact on evolvability and computational power. Those can be grouped in three macro-categories:

- Intrinsic: this is related to internal properties of the molecules that compose the material, for example the type of used particles and their composition. This decides the physical properties that may be available to be exploited, e.g., conductivity, charge, etc.
- External/Environmental: external stimuli that influence the material properties, such as current, temperature, light. Those can be of two types: controllable, e.g., evolved, or non-controllable. External inputs may have an impact and change the physical state of the material temporarily or permanently.
- Construction: those are properties that are decided when the system is built and cannot be changed afterwards. As such, they may be said to be both external, i.e., construction choices, and internal, as they influence the intrinsic physical properties of the material, e.g., concentration of molecules, type of nanotubes (metallic, semi-conducting), electrodes material, size and pitch.

As there are several variables to be explored, it is reasonable to acquire a better understanding of how the most relevant parameters impact the computational power of materials. The more we know about materials, the better they can be used for computations (or any other purpose we may want to use them for).

This paper, which serves as a work-in-progress report, is organized as follows: Section 2 describes the investigated material and hardware platform. Section 3 relates the work to dynamic complex systems and chaos. In Section 4, the experimental setup is described and Section 5 presents the

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results and discussion. Section 7 concludes the paper together with planned future work.

II. MATERIAL AND HW PLATFORM

The current experiments are performed on a blob of single-wall carbon nanotubes (SWCNT) mixed with polybutyl methacrylate (PBMA) dissolved in anisole (methoxy-benzene). The material samples, supplied by Durham University, are prepared on 4x4 grids of gold micro-electrode arrays with pads of 50µm and pitch of 100µm. The preparation is done by dispensing 20µL of material onto the electrode area (CNT concentration 0.53% of weight). This is baked for 30min at 90C; the solvent dries out and leaves a "thick film". The substrate is cooled slowly over a period of 1h. This process leaves a variable distribution of nanotubes across the electrodes. Carbon nanotubes are 30% conducting and 70% semi-conducting, while PBMA creates insulation areas within nanotube networks, which may allow non-linear current versus voltage characteristics.

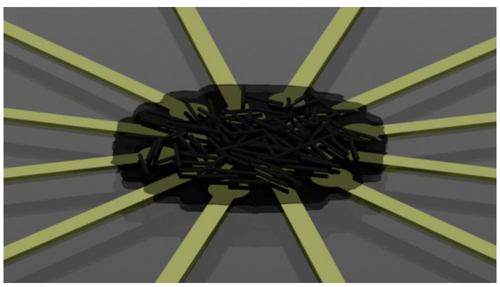

Figure 1. Sketch of nanotubes dispersed over electrodes.

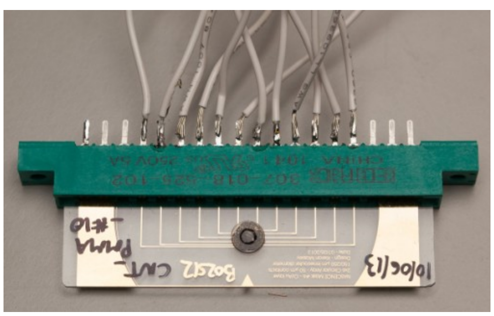

Figure 2. Electrode array slide plugged into connector.

A sketch of randomly dispersed nanotubes over gold electrodes on a glass slide is shown in Figure 1. The glass slide on which the material and electrodes are placed is plugged into a connector as represented in Figure 2. Such connector is attached to a custom built hardware board called Mecobo [13] (designed and built at the Norwegian University of Science and Technology), which is connected to a host PC via USB. Such platform can be accessed remotely over the internet by a Thrift server. Figure 3 shows a Mecobo board with a connected material slide. An overall block diagram of the system is presented in Figure 4. Mecobo serves as interface for computer-controlled evolution of configuration signals (analog or digital) to stimulate the nanomaterial to solve computational problems. For more details on the Mecobo platform see [13].

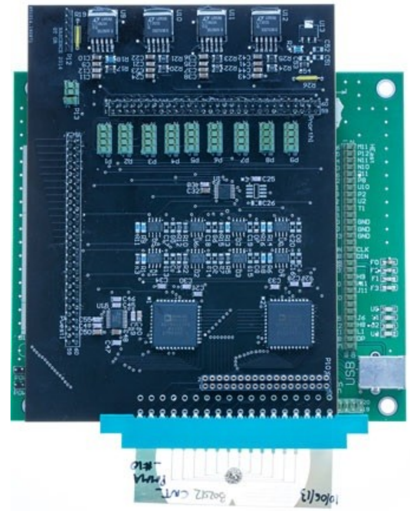

Figure 3. Mecobo interface between nanomaterial and PC.

In a typical experiment, the overall goal is to solve a computational task. Output signals are sampled from the material by the board and returned to the host computer which executes an evolutionary algorithm and calculates the fitness. The maximum sampling frequency is 50KHz. The input signals may be static voltages or square waves ranging between 400Hz and 25MHz. As the material is treated as a black-box, the input stimuli are used to exploit the underlying physics of the material blob. On the other hand, if we want to unveil the computational power of materials, how to better exploit them, and how to use them to solve problems of scaled-up complexity, a different approach is needed. As such, in the experiments herein we connect material slides to a Hewlett Packard 33120A 15MHz function / arbitrary waveform generator (used as input) and an Agilent 54622D 100MHz mixed signal oscilloscope (used as output).

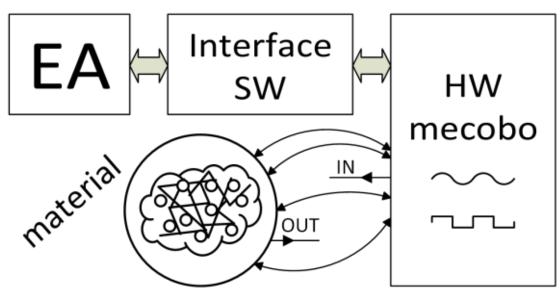

Figure 4. Experimental system block diagram.

III. COMPLEX DYNAMIC SYSTEMS AND CHAOS

Carbon nanotubes randomly dispersed in polymer solutions may be considered as a complex dynamic system where a huge number of tiny elements (nano-molecules)

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interact at a local level and exhibit different emergent dynamics [14]. Such an emergent process cannot be understood by describing one of its parts alone but must be considered together with the massively parallel interactions among its parts. The idea of complex dynamic systems is connected with the notion of “edge of chaos” [15] [16], which may indicate maximum complexity and computational power. Computation may be said to occur in the vicinity of a phase transition between order, i.e., little dynamics / information processing and high memory / structure preservation, and chaos, i.e., no memory and plenty of dynamics. It may be argued that in order to have any complex computation, a balance between order and chaos needs to exist, i.e., edge of chaos. Computation at the molecular level, i.e., computation-in-materio, may be able to produce considerably rich dynamics as the very essence of the material physics is exploited. This may allow to abstract computational properties and analyze the dynamics of the investigated substrates as trajectories and attractor basins [17].

IV. EXPERIMENTAL SETUP

Evolving solutions to computational problems in the material requires interfacing to a computer (EA). Such interface is typically provided by the Mecobo board. However, when it comes to understanding the underlying properties of the material and relative responses, it may be necessary to use specific electronic test instruments, i.e., oscilloscopes and signal generators.

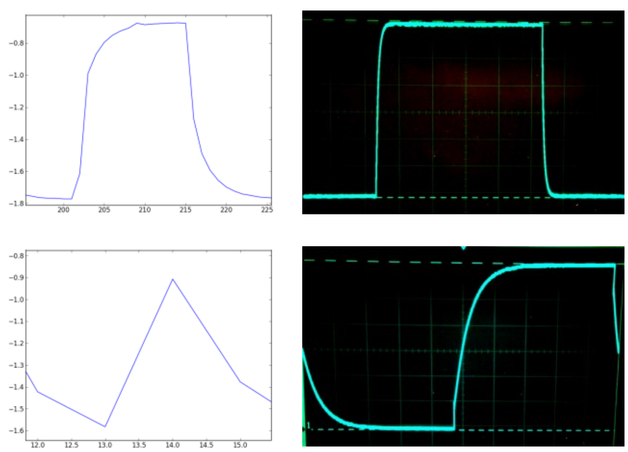

Figure 5. Mecobo (left) vs. oscilloscope (right) at 1KHz (top) and 10KHz (bottom). Input ±3.3V, duty cycle 50%.

Figure 5 presents the same square wave (±3.3V, duty cycle 50%) at a frequency of 1KHz (top) and 10KHz (bottom), sampled with Mecobo (left) at a frequency of 25KHz and probed with the oscilloscope (right). It is visible that the material may show a charge / discharge transition, but the level of details is partially lost with Mecobo. As the operating input frequency may range between 400Hz and 25MHz, while the maximum sampling rate is 50KHz, it is clear that physical properties of the material need to be investigated with an oscilloscope. On the other hand, when solutions ought to be discovered by an evolutionary algorithm, Mecobo acts as an interface, being able to produce different inputs, i.e. analog and digital, on different pins and read outputs at the same time.

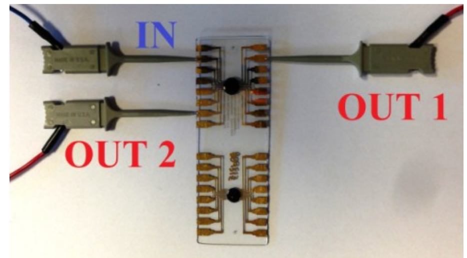

Figure 6. Schematics without Mecobo.

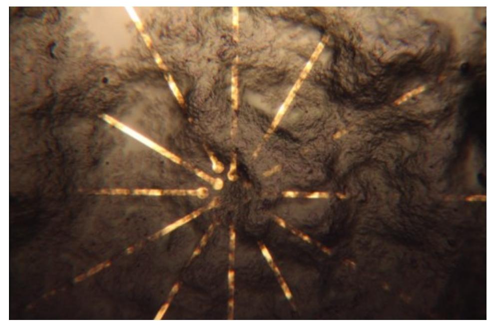

Figure 7. SEM image of gold electrode arrays with different coverage of nanotubes. Adopted from [8].

The chosen experimental setup is shown in Figure 6, where the input probe (from the signal generator) is placed on pin #2 (IN) and the two output probes (to the oscilloscope) are connected to pins #9 (OUT1) and #7 (OUT 2). The input / output pins have been chosen as there is the same electrode distance between gold pads within the material blob. Coverage of gold electrodes with randomly dispersed nanotubes varies and some of the electrodes may even be left with little or no coverage, as visible in the Scanning Electron Microscope (SEM) image in Figure 7.

One of the expected results is to achieve different responses on different output pins, as the material from a macroscopic point of view has the following properties:

- Varying capacitance between pin pairs;
- Varying inductance between pin pairs;
- Varying induced magnetic field, inducing current in other parts of the material;
- Varying resistance between pin pairs;
- Varying metal/semiconductor junctions, e.g. different coverage of carbon nanotubes on gold probes.

V. RESULTS AND DISCUSSION

Even if a single square wave input signal is used, the resulting output shows a rich variety of behaviors, more than

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what may be achieved by a single static voltage or by a sinusoidal wave. As such, square waves may be better suited to penetrate the material and exploit the nanotube sub-networks, which may be particularly sensitive to different frequencies.

Figure 8 presents the experimental results. In particular, Figures 8(a) show several snapshots of the material response on two different pins at different frequencies, ranging from 1KHz (Figure 8a1) to 14MHz (Figure 8a12). At 1KHz the signals may seem similar (a1), where the material charges-up and subsequently discharges, but at a zoomed-in resolution (a2) a voltage spike is visible on the second probe which is not present on the first probe. This is better visible at 5KHz (a3), 30KHz (a4) and 100KHz (a5), where it is possible to notice that on the rising front there is a sudden voltage increase/drop, as the material behavior is "supercapacitor-like". Starting from 500KHz (a6), which is also zoomed-in (a7), the second probe signal is similar to a square wave (most of the harmonic frequencies are passed) while the first probe acts more like a filter. In both cases, there is a resonance phase which results in a deterministic yet semi-chaotic waveform. This may be the effect of some conducting sub-networks in the material that are enabled at specific frequencies and disabled at others. At 2, 5 and 8.5 MHz the measured voltage decreases while frequency increases. At 10MHz (a11) a strange phenomenon is observed where both signals (it is more noticeable on the first) have a voltage increase, probably due to a feedback-effect (some frequencies are fed again into the material by some nanotube sub-networks). At 14MHz (a12) the signal on the second probe is sinusoidal, i.e., only one harmonic frequency is present. As such, it may be concluded that with a single square wave input it is possible to observe a rich variety of behaviors while the frequency spectrum is traversed.

As the system produces uniform, stable and semi-chaotic behaviors, it is of particular interest to visualize input-output responses and output-output relations, as to better understand traversed trajectories and attractors. For this purpose, XY plots are shown in Figure 8b, where OUT1 is plotted against OUT2 and Figure 8c, where IN is plotted against OUT1. In Figure 8b1, some orbits are present at 30KHz. Similar orbits are visible at 60KHz (b2) and 100KHz (b3), moving towards opposite corners to those where the impulse is. After each impulse, there is a semi-chaotic orbit which relaxes before the next impulse arises, as the semi-chaotic behavior is annihilated by the lack of energy in the material, until the next impulse. This may suggest that chaotic behavior may be present, yet particularly difficult to observe.

Finally, we present XY plots between input and output, which represent the phase space of the system (input-output pin pair). Figure 8c1 is registered at 350Khz. Several oscillating orbits are present, which are zoomed-in at 2MHz (c2). Same effect is observed for frequencies up to 5MHz (c3) while for frequencies around 10MHz and higher we observe a hysteresis loop which may indicate that some saturation may have been reached in the material. Some sort of non-linearity seems present, which is always a good indicator that the system may achieve chaotic behavior.

VI. Conclusion and Future Work

In this paper, we presented interesting properties of nanocomposites of single-wall carbon nanotubes and polymers. Such material blobs are investigated within the NASCENCE projects as one of possible novel computational substrates. Previous work has presented proof of concept for the solution of several problems, where the material blob was used as a black-box and interfaced to a computer running EAs through a custom developed board. Our approach was intended for investigating different behavioral responses when the material is stimulated with square wave voltages at different frequencies, with the goal of detecting non-linear and chaos-like behaviors. As such, signal generator and oscilloscope's probes were connected to the material gold electrodes. This was done to understand underlying physical responses and suitable signal frequencies able to show computationally rich behaviors. The work in progress results are promising as a single square wave signal has been shown to produce a variety of responses dependent on pins and frequencies. Phase space plots have been presented with orbiting trajectories alternated to relaxed transients. Responses that may be exploited for evolution have been identified at rather low frequencies, in ranges below MHz.

As future work we will continue our investigation to search for interesting responses and new methods for their analysis, in particular with the goal of determining whether chaotic behavior is present. The presence of chaos may be considered a benefit of the used computational materials, as the described theory on the computation at the "edge of chaos" may be plausible for computation at the molecular level, where the low physics of material are exploited.

Another future direction is the modeling of different materials at different abstraction levels. Currently, cellular automata (CA) models of materials are considered. Such an approach has the advantage of representing different computational behaviors as trajectories and attractor basins, allowing measurements on computational complexity and computational power of materials.

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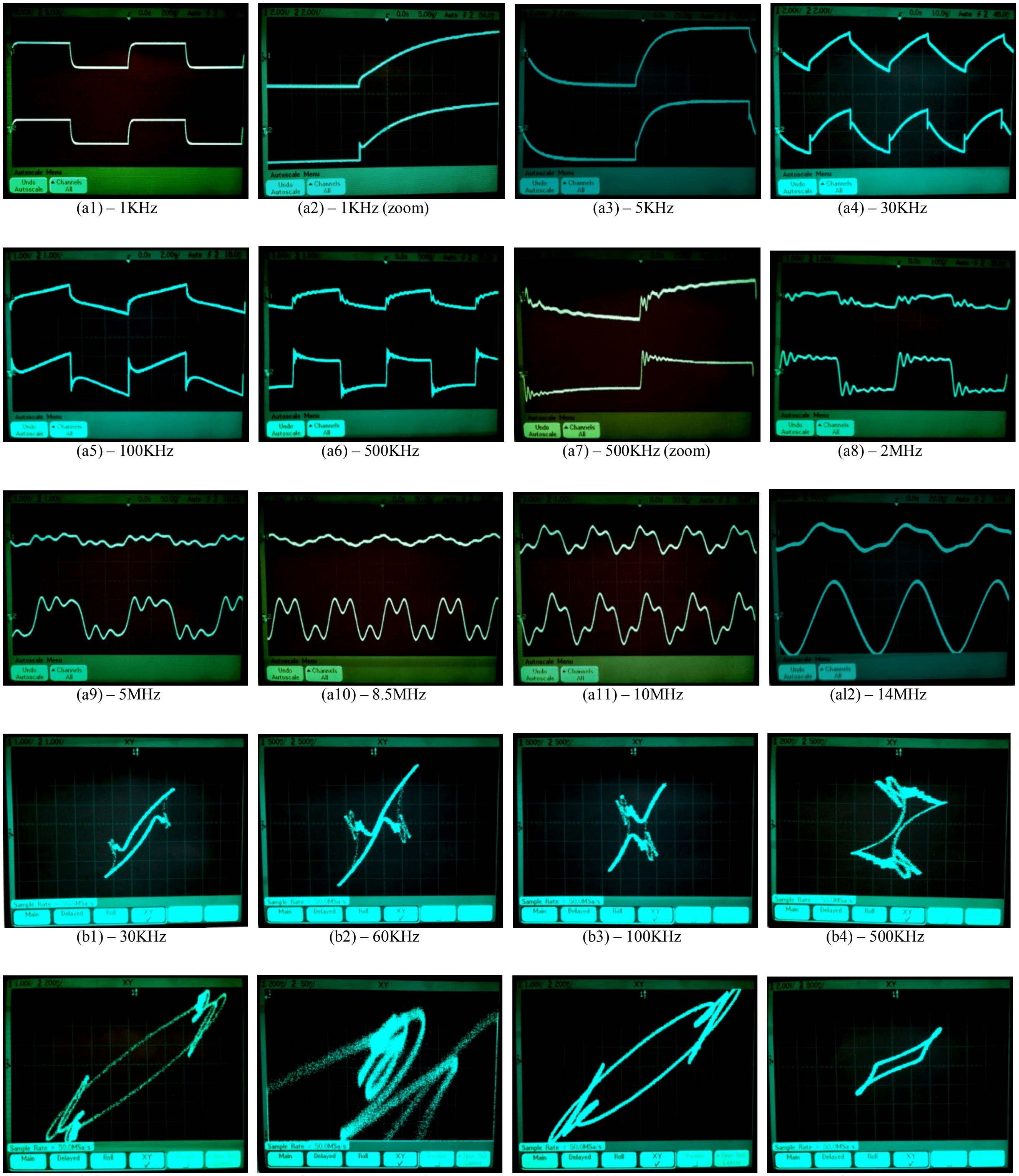

(a1) – 1KHz (a2) – 1KHz (zoom) (a3) – 5KHz (a4) – 30KHz

(a5) – 100KHz (a6) – 500KHz (a7) – 500KHz (zoom) (a8) – 2MHz

(a9) – 5MHz (a10) – 8.5MHz (a11) – 10MHz (al2) – 14MHz

(b1) – 30KHz (b2) – 60KHz (b3) – 100KHz (b4) – 500KHz

(c1) – 350KHz (c2) – 2MHz (zoom) (c3) – 5MHz (c4) – 10MHz

Figure 8. Oscilloscope screenshots.
(a) Voltage responses on 2 different pins with input square wave at different frequencies.
(b) XY plots, X (OUT1) is plotted against Y (OUT2) at different frequencies.
(c) XY plots, X (IN) is plotted against Y (OUT1) at different frequencies.

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