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STATISTICAL ANALYSIS OF WEAKEST LINK IN CHAINS OF MAGNETIC PARTICLE CARRIERS FOR APPLICATIONS IN PRINTING BIOCHEMICAL ARRAYS

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INTRODUCTION: Magnetic particle chains have been studied in the past as a means for delivering magnetic particles to surfaces. In situations where the magnetic energy of the particles is comparable with the energy of thermal fluctuations, chain structures have been analyzed using statistical methods [1]. For relatively large diameter particles (i.e. greater than 100-nm), magnetic energy dominates thermal fluctuations, and therefore the deterministic approaches taken by Harpavat [2] and Alward [3] are justified. Previous authors have analyzed the force between each joint in a linear chain of permeable magnetic spheres to determine the weakest link [2,3]. In both these approaches, the particles in the chain were magnetized by a magnetic source at one end without considering the saturation magnetization of the particles. By contrast, this paper considers a situation in which the external magnetic field completely saturates the particles, and the weakest link is determined for a chain in contact with a magnetized substrate at both ends.

The main motivation for this analysis is to better understand the conditions that promote deposition of a specific number of particles onto a magnetized substrate. The ability to control the number of particles deposited has great potential for biochemical printing applications, where the goal is to control the amount of material deposited and maximize the density of the array. An example of an array that is printed with labeled magnetic particles is shown in Fig 1.

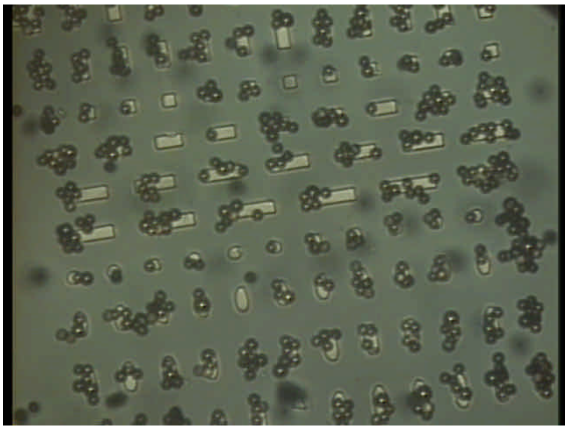

Fig 1: Magnetic particles (5 µm diameter) deposited onto an array of magnetic islands of different shapes and sizes magnetized in planar direction.

In this paper, we consider a situation in which a magnetic island, whose magnetization is perpendicular to the substrate, interacts with a chain of magnetic particles held by a larger magnet at the opposite end. Both the island and external magnets are modeled as cylindrical bodies that are magnetized along their axis perpendicular to the substrate and separated by the length of the chain. It is also assumed that all particles in the chain are magnetized to saturation by external magnetic fields directed along the chain axis.

In an attempt to model a more realistic situation, the particles are treated as having random saturation magnetization and random sizes. The distribution of radii is chosen to be consistent with currently available materials, whereas the distribution of magnetic moments is chosen to be log normal according to a frequently used assumption. In addition, several assumptions are made to simplify calculations. One is that the presence of magnetic particles does not influence the magnetization of the substrates. This assumption is justified for substrates composed of a relatively hard magnetic material. Another assumption is that the particles are treated as constant dipoles.

This paper will be organized as follows. First, a brief overview of the computational method will be provided. Then, calculation results for the deterministic case will be shown and general trends described. Subsequently, the radii and magnetic moments of the particles are given random probability distributions, and the expected force and standard deviation at each joint in the chain will be calculated for varying circumstances. With the breaking range of a joint considered to be within one standard deviation of the expected value, the question of how reliably the particles are deposited will be answered. Finally, a brief conclusion will be provided.

COMPUTATIONAL METHOD: The force on a magnetic dipole of moment *m* due to a magnetic field with flux density component in the z-direction denoted by B_z is given by

$$F = -m\frac{\partial B_z}{\partial z} \qquad (1)$$

Assuming that saturation flux density of a cylindrical magnet that is magnetized along its own axis is B_s, then the z-component of the flux density of this magnet along its axis is

$$B_z(z) = \frac{B_s}{2}\left(1 - \frac{z}{\sqrt{z^2 + r^2}}\right) \qquad (2)$$

where r is the magnet's radius whose length is assumed to be many times greater than its radius, thereby allowing us to neglect the field contribution due to the furthest pole face of the magnet. In this paper, the magnetic field of the island B_{isl} and the magnetic field of the magnet B_{mag} will be computed according to (2).

A chain of magnetic dipoles is aligned along the z-axis, attached to the magnet at the $z = 0$ end and to the magnetic island at the $z = L$ end. The force that the magnet exerts on the entire chain of magnetic dipoles and island (i.e. the force on the 0^{th} joint in the chain) can be found from (1) and (2) as follows:

$$F_0 = -q_{isl}B_{mag}(L) + \sum_{i=1}^{N} m_i \frac{\partial B_{mag}(z_i)}{\partial z} \qquad (3)$$

where q_{isl} is the magnitude of the effective magnetic charge on the pole face of the island, m_i is the magnetic moment of the i^{th} particle, and z_i is the z-position of the center of the i^{th} particle of radius r_i given by:

$$z_i = -r_1 + \sum_{j=1}^{i} 2r_j \qquad (4)$$

Note that in deriving (3) it was assumed that the island diameter is much smaller than the magnet diameter justifying the use of an effective magnetic charge representing the effect of the island.

To determine the force at any joint in the chain, one needs also to account for forces between magnetic particles located on opposite sides of the joint. The interaction force between the i^{th} and j^{th} magnetic dipoles in the chain is given by:

$$F_{ij} = -\frac{m_0}{2p} m_i m_j \frac{\partial}{\partial z_i} \frac{1}{(z_i - z_j)^3} \qquad (5)$$

Using (1-5), the force at the n^{th} joint in the chain can be calculated:

$$F_n = F_0 - \sum_{i=1}^{n} m_i \frac{\partial B_{mag}(z_i)}{\partial z} - \sum_{i=n}^{n} m_i \frac{\partial B_{isl}(z_i)}{\partial z} + \sum_{i=1}^{n} \sum_{j=n+1}^{N} F_{ij} \qquad (6)$$

The force at each joint in the chain is thus computed, first deterministically, and then with statistical variations for 1000 trials using randomly generated values of particle radius and magnetic moment. The particle radius is treated as a random variable with uniform distribution between 90-110% of a chosen mean value, while the magnetic moment is treated as a random variable with log normal distribution and with 90% of its probability density occurring between 0.85 and 1.2 times the expected value. Using this method, the expected force and standard deviation is calculated for each joint and the weakest links are determined.

RESULTS: The above computational method for finding the average weakest link in a chain was implemented with MATHCAD software. Magnetic flux densities of the magnetic substrates are chosen to be in the range of 0.2 – 1.0 Tesla, which is consistent with the remnant magnetization of available magnetic materials, such as Fe and Co [4]. The diameter of the island was fixed at 1-ìm, while the particle and external magnet diameters are referenced against the island diameter. In this paper, the particle diameters were limited to a range of 0.1 to 10.0 times the island diameter, and the external magnet's diameter in most cases was limited to a range of 100 to 1000 times the island diameter. These values were chosen because they are experimentally realistic and consistent with available materials and methods.

Current photolithographic tools can produce 2-D patterns in thin films in the sub-micron range, and external magnets with millimeter and sub-millimeter diameter are relatively easily to manufacture. Additionally, magnetic particles in the micron range are currently being used in various biochemical labeling and bio-sensing applications.

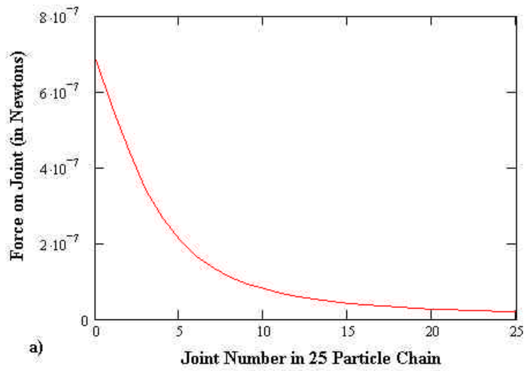

Fig. 2: Illustration of the weakest link in a 25-particle chain where the external magnet diameter is 100 times the island diameter and both magnetic substrates have 1 Tesla flux density. The particle diameter is 10 times the island, and the minimum force occurs at the joint in contact with the island.

The weakest link in the chain was first calculated deterministically, and certain trends were observed for varying chain lengths, particle and external magnet sizes. For chains composed of large particles with diameter exceeding 10 times the island's diameter, for example, the island's magnetic field gradient is too weak to retain massive particles. In these circumstances, the weakest joint is frequently at the island surface, as is shown in Figure 2.

For chains composed of very small particles with diameter less than 0.1 times the island diameter, the gradient due to the island is felt much more strongly throughout the chain. In these circumstances, the weakest joint is frequently at the external magnet surface, as shown in Fig 3.

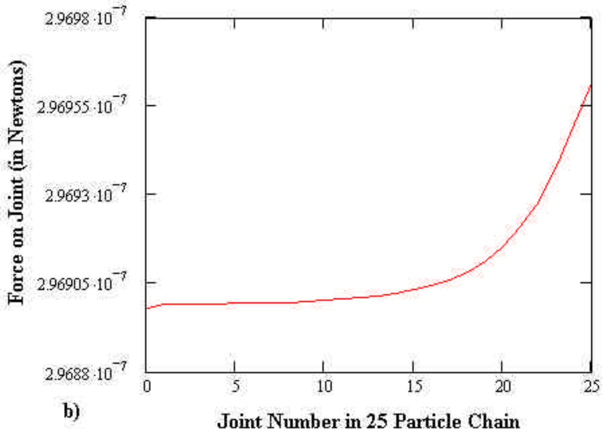

Fig. 3: Illustration of the weakest link in a 25-particle chain where the external magnet diameter is 100 times the island diameter and both magnetic substrates have 1 Tesla flux density. The particle diameter is 0.1 times the island, and the minimum force occurs at the joint in contact with the external magnet (i.e. the 0^{th} joint).

In contrast, situations in which particles and island have equal diameters show that the weakest link in the chain is frequently one of the interior joints. The reason the break occurs in the interior is that the island exerts a stronger force on the nearest few particles due to its similarity in size. However, the island's field gradient decreases very quickly, in contrast with the external magnet's field gradient, which decreases slowly. As a result, it can be seen intuitively that the energy minimum occurs at a joint closer to the island side.

Among the joints closest to the island, the exact weakest link is strongly influenced by the length of the chain as well as particle and external magnet diameters, as is shown in Fig 4. For example, in 10-particle chains with equal particle and island diameters, the weakest link is usually within the first three joints from the island side. In short chains, a small magnet can exert greater forces on each particle than can a large magnet, due primarily to the fact that a smaller magnet has stronger local magnetic field gradient.

For long chains, however, the field gradient due to a small magnet dies out very quickly. A large diameter magnet, by contrast, has a slowly decreasing magnetic field gradient, which exerts a strong influence much farther down the chain, as is shown in Fig 4b. A general conclusion for printing applications, which requires printing relatively few particles onto a magnetic island, would be that a smaller magnet should be used with shorter chains and a larger magnet with longer chains.

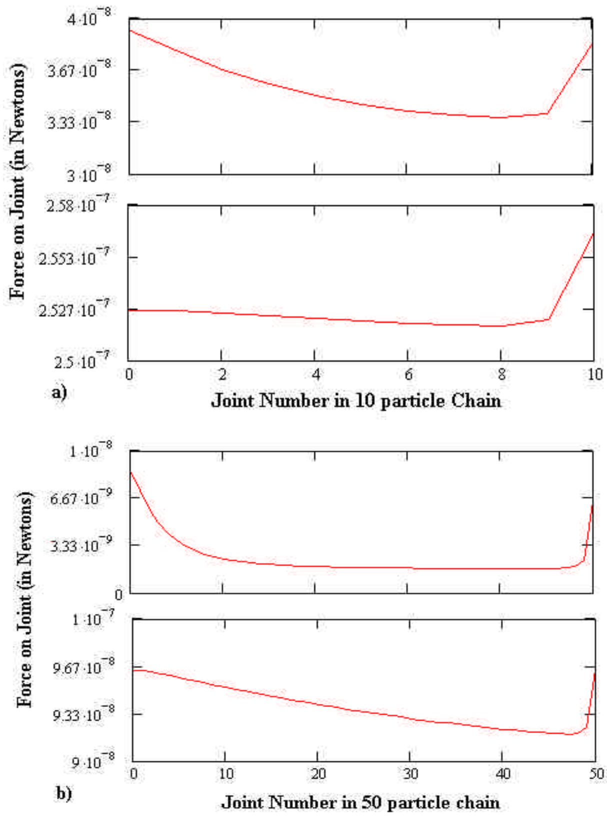

Fig. 4: Illustration of the effects of varying external magnet diameter on a) 10 particle chains and b) 50 particle chains with equal particle and island diameter and magnetic field densities of both substrates equal to 1 Tesla. The top graph for a) and b) represents the effect of a small diameter external magnet (10 times the island diameter), whereas the bottom graph represents the effect of a large diameter magnet (100 times the island diameter).

Next, the weakest link in the chain was computed probabilistically to determine how reliably the chain breaks at a specific joint. The particle radii and magnetic moments were treated as random variables, and the expected force and variance were calculated at each joint. The breaking range at each joint was designated to be within one standard deviation of the expected value, as is shown in Fig 5. Using these ranges, it is possible to determine not only the weakest joint, but also if the breaking range of another joint intersects the breaking range of the weakest joint. If the two ranges intersect, then the chain may break at either joint when a force within that range is applied.

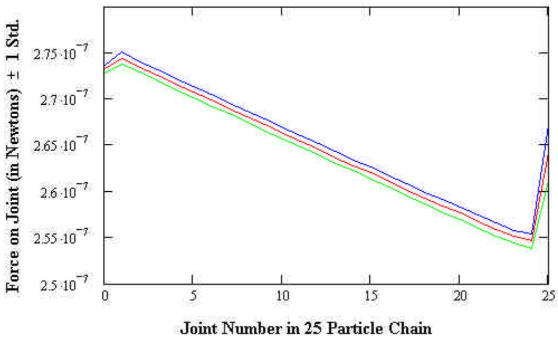

Fig. 5: Illustration of the force on each joint in a 25-particle chain (red), as well as one standard deviation to the plus (blue) and minus (green) sides. The particle and external magnet diameters are 4 and 500 times the island diameter, respectively; and both magnetic substrates have1.0 Tesla magnetic field density. There is clearly a minimum at the joint between the first and second particles from the island side.

In general, it is beneficial to know what circumstances are conducive to printing 1-4 particle chains onto a magnetic island.

Table 1. Number of Particles Deposited with Varying Parameters.

Trial	P:M	Chain	B_{isl}	B_{mag}	Part.
1	5:250	14-20	1.0	1.0	1
2	4:200	8-17	0.75	1.0	1
3	3:200	2-14	0.4	1.0	1
4	2:200	3-12	0.2	1.0	1
5	5:500	17-45	1.0	1.0	1,2
6	4:500	7-28	1.0	1.0	1,2
7	4:500	20-58	0.5	1.0	1,2
8	3:500	4-32	0.5	1.0	1,2
9	3:1000	6-47	0.25	1.0	1,2
10	2:200	13-38	0.2	1.0	1,2
11	5:1000	46-77	1.0	1.0	1,2,3
12	4:500	29-49	1.0	1.0	1,2,3
13	3:500	33-65	0.5	1.0	1,2,3
14	3:100	29-38	0.5	1.0	1,2,3
15	2:200	39-63	0.2	1.0	1,2,3
16	2:200	12-25	0.4	1.0	1,2,3
17	5:500	72-78	1.0	1.0	1,2,3,4
18	4:500	50-66	1.0	1.0	1,2,3,4
19	3:500	66-87	0.5	1.0	1,2,3,4
20	2:200	25-45	0.4	1.0	1,2,3,4
21	5:500	3-36	0.5	1.0	0,1
22	5:500	37-47	0.5	1.0	0,1,2
23	4:200	4-22	0.5	1.0	0,1
24	1:200	50	1.0	0.5	Any
25	0.5:200	50	1.0	1.0	Any

With all the potential variations in particle size, chain length, island and magnet radii and field densities, it is unclear how to demonstrate the effects of all these variables in a graph. Therefore, Table 1 will be used to represent some of the circumstances in which only a few particles will be deposited on the magnetic island substrate. In Table 1, the variable *P:M* represents ratio of particle to external magnet size, *Chain* is the chain length in terms of number of particles, B_{isl} and B_{mag} are the magnetic field densities of the island and external magnet in Tesla, and *Part* represents the number of particles remaining on the island given the intersecting probability ranges. The table can be read as follows. In trial 6, when the particle is 4 island diameters, the external magnet is 500 island diameters, and the magnetic field density of the island and external magnet are both 1.0 Tesla, then the chain will break at either the first or second particles away from the island for chain lengths between 7 and 28 particles long

CONCLUSIONS: A set of chains attached to a large magnet can be idealized as a "magnetic brush". If the chain bristles of the brush come into direct contact with a magnetic island whose diameter is on the same order as the particle, then in some situations a few particles will remain attached to the islands when the brush is pulled away. Assuming all parameters including chain length, particle size, magnet diameter and magnet strengths can be tuned appropriately, this magnetic brush may potentially be used to paint a specific number of particles onto an island.

For sufficiently long chains with average particle diameter between 2 and 5 times the island diameter, it was found that the chain consistently deposited between 1 and 4 particles onto the islands. Such situations are considered to be desirable; moreover, it is shown that system parameters can be varied to make extreme situations, in which a large number of particles or no particles are deposited, statistically unlikely.

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